HPCAT

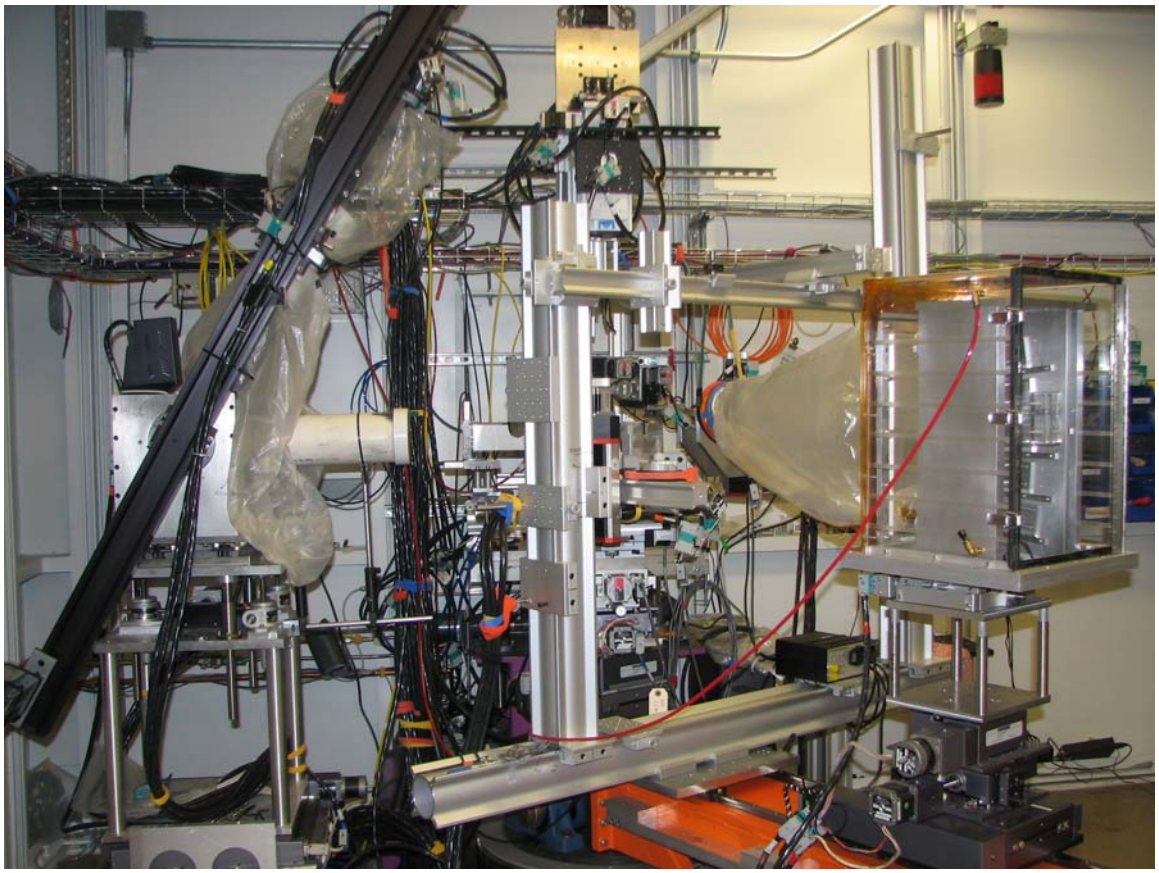
16 IDD

User Manual

CARNEGIE INSTITUTION FOR SCIENCE

High Pressure Collaborative Access Team
Advanced Photon Source

16 IDD User Manual



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Chapter

1

About 16 ID-D

Beamline description

The The HPCAT 16ID-D beamline is dedicated to x-ray scattering and spectroscopy research of materials under high pressure, typically in diamond anvil cells (DAC). With beams of 2meV energy resolution at ^{57}Fe energy of 14.413keV, nuclear resonant techniques are used for determining phonon density of state and Mössbauer effect for Fe-containing samples at high pressures. With beams of 1eV energy resolution, a high efficient instrument for x-ray inelastic scattering (x-ray Raman) provides information of charge dynamics and chemical bonding at high pressures. The 16ID-D station has also a setup of emission spectrometer, measuring the details of fluorescence signals for information of spin state and structures of valence electrons at high pressures.

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Major ID-D features

Feature	Description
Source	Dual undulators Type A, single or in tandem mode
Monochromator	Oxford Diamond (1 1 1) DCM
Energy Range	5-25keV
Beam Size and Focusing Optics	35 (V)x 50 (H) μm with 1 meter long KB mirrors 10 (V)x 10 (H) μm with 200mm long KB mirrors or combine 1 long KB mirror with 1 short KB mirror
Flux at Sample Position	NRS: ~$1x10^{9}$ ph/s, 2meV energy solution Others: ~$2x10^{12}$ ph/s flux based on using 1 meter long KB mirrors
Established Techniques	Nuclear Resonant Inelastic X-ray Scattering (NRIXS) Nuclear Forward Scattering (NFS) Inelastic X-ray Scattering (IXS) X-ray Raman Scattering (XRS) Resonance/X-ray Emission Spectroscopy(R/XES) Partial Fluorescence Yield X-ray Absorption Spectroscopy (PFY-XAS) X-ray Fluorescence Spectroscopy (XFS)
Detectors	100K Pilatus detector, Avalanche Photo Diode (APD), AmpTek
Support Equipments	Cryostats for XES and NFS, online Ruby system

Chapter

2

Troubleshooting

Data collection computer crash

If the data computer crashes or doesn't response during the experiment, please restart the computer and follow steps in "LOGIN" and "HOW TO START EPICS INTERFACE" section in Chapter 3.

Bluediamond

Sluggish response

The real-time data display is basically relying on the data in/out control routine which uses EPICS channel access method; therefore this software becomes sometimes sluggish depending on the local network traffic status, which may vary station by station even within the same sector and at the same time. Many bugs have been reported by users for past cycles; and most of them were fixed in the latest version (2010 March).

No response and Restart

If the software is waiting for the input PV values updated as a scan started and if there is no update in the PV, it may wait for the input signal update forever. There is no feasible timeout routine to reset this error, according to the writer of software. This error is, however, often caused by the errors involved in EPICS Scan procedures, which can be caused by a mistake in the input PV values (e.g., incorrect scan range) and may need to acknowledge the error or reset it on the MEDM interface (not on the Bluediamond).

If you need restart Bluediamond, firstly you need press "Ctrl+Alt+Del" to start the Task manager under Windows, then kill the Bluediamond in the Application. Secondly, follow steps in "BLUEDIAMOND" section in chapter 3.

IDL scanSee Software is not working

If ScanSee crashs or has no response, please close it and restart it following steps in "IDL SCANSEE SOFTWARE" section in Chapter 3

Losing beam intensity

One of the most frequent causes of beam intensity decrease in the experimental hutch is accidental bump into the pinhole, if so, please check the Y and Z positions of pinhole and the sample alignment.

If it is not the pinhole problem, there are several possibilities.

1) If the APS is running at decay mode (ring current decreases gradually from 100mA to 80mA), you will see intensity decrease slowly , that is normal, so you don't do anything. The intensity will come back after re-injection.
2) If there is a beam lost, the DCM need time to warm up, during warming up period, the intensity will drop, to get intensity back, we need adjust DCM pitch to get maximum intensity. After adjust pitch, beam position will also be changed, so we need steer beam positions, please follow steps in "STEERING BEAM PROCEDURES" in chapter 3.
3) If the intensity changes suddenly, you can look at APS beam position monitor to check source beam positions and compare it to those values we print out. If you see big change, please let beamline scientist know, then we need call floor coordinator to ask APS control room to steer beam.

Chapter

3

Beamline operations

Login

Both beamline control computer and data analysis computer (Windows XP Professional operating systems) has identical login id and password for users:

login: **16idd_user**
password: **idduser@16**

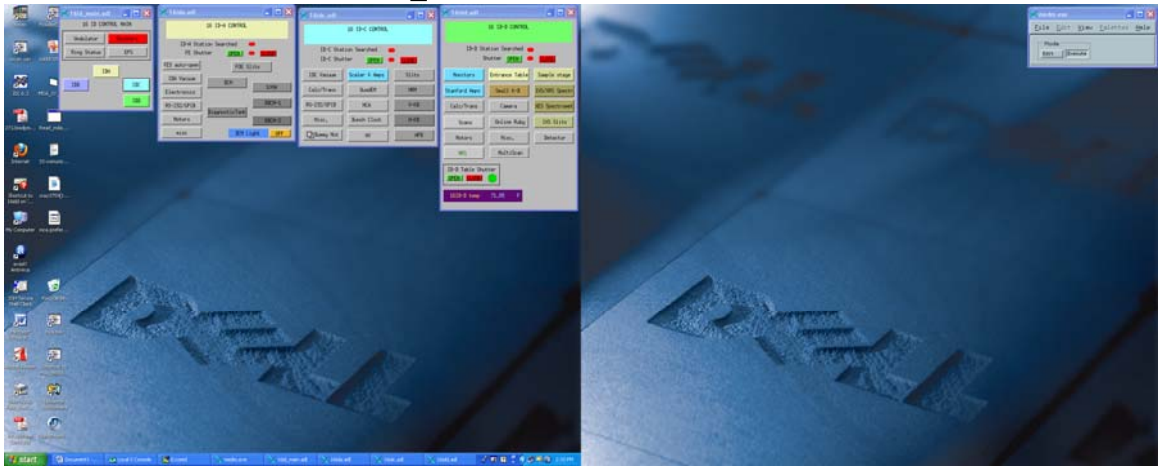
This login id and password will be required when re-logging in the computers (e.g., after rebooting the operating system) and also valid to access network data folder \\hpcat21\16idd.

How to start EPICS interface

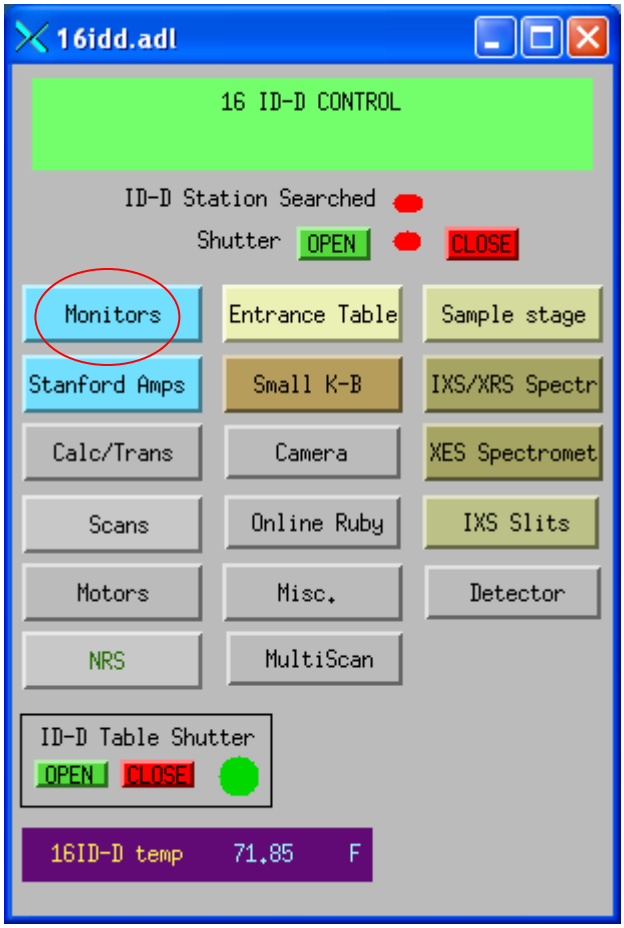
1. double click “MEDM”

2. change medm.exe from “Edit” to “execute”

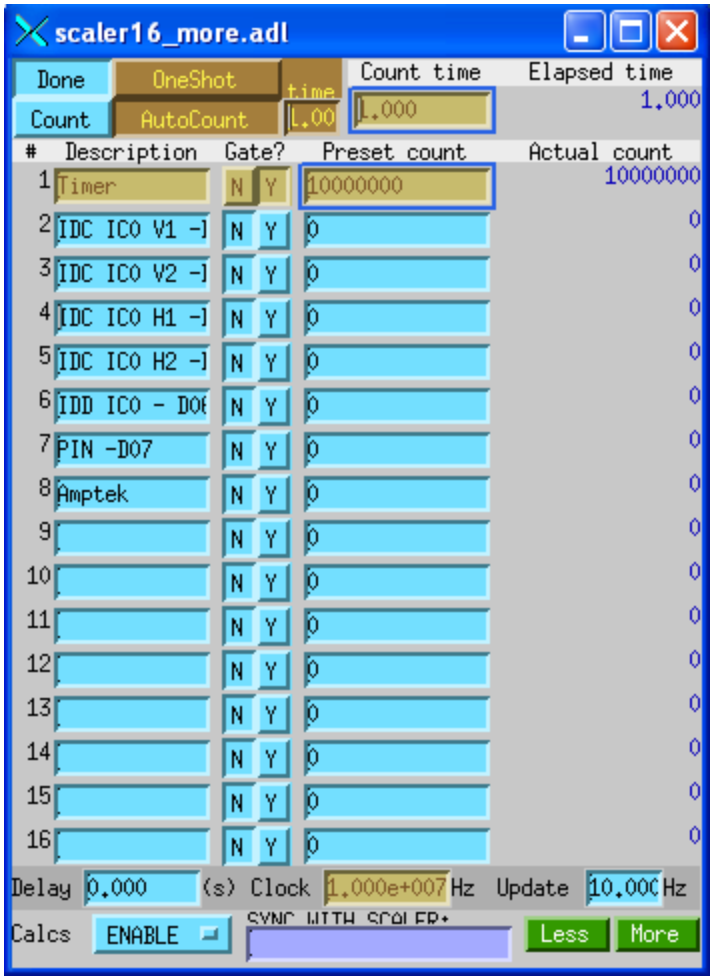
3. click “IDA” “IDC” “IDD” from 16id_main.adl



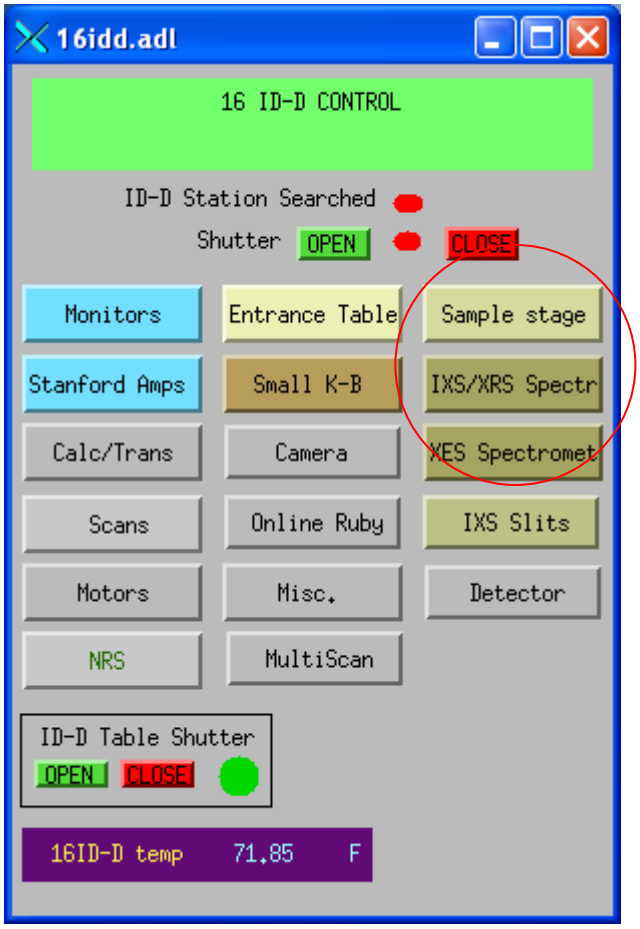
4 click “Monitors” from 16idd.adl



then scaler window pops up



5. Depends on experiment, you can open sample stage, IXS/XRS, XES spectrometer from 16idd.adl

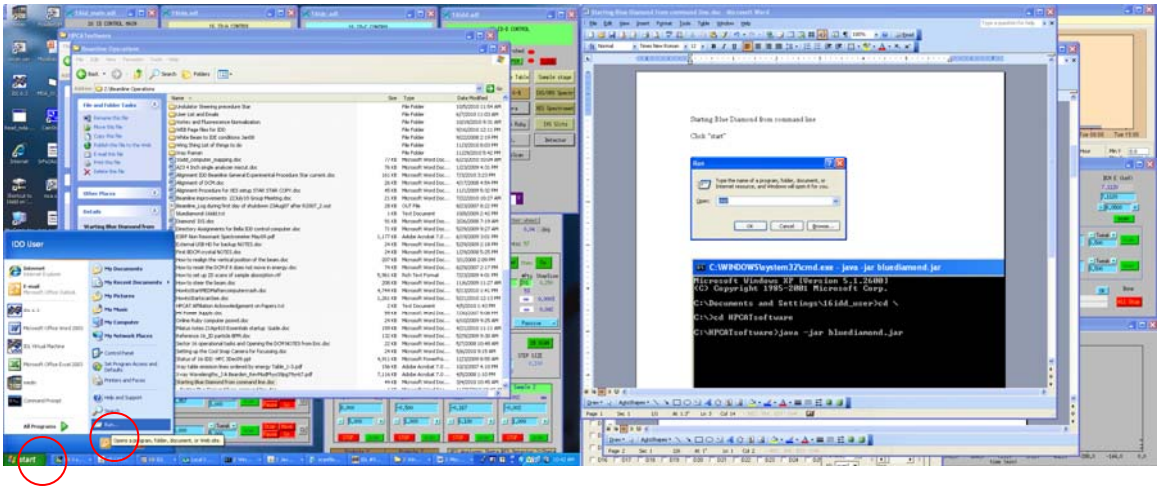


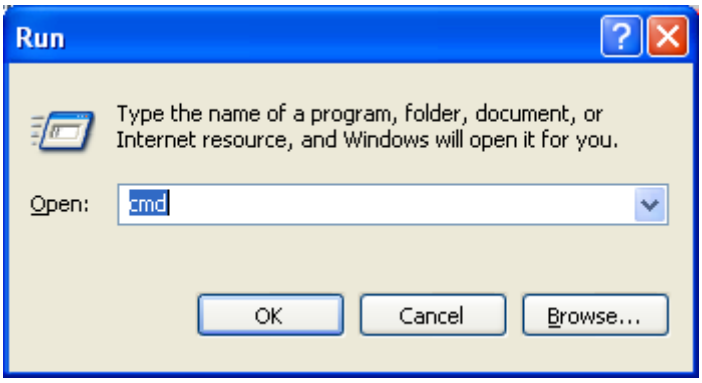
Bluediamond

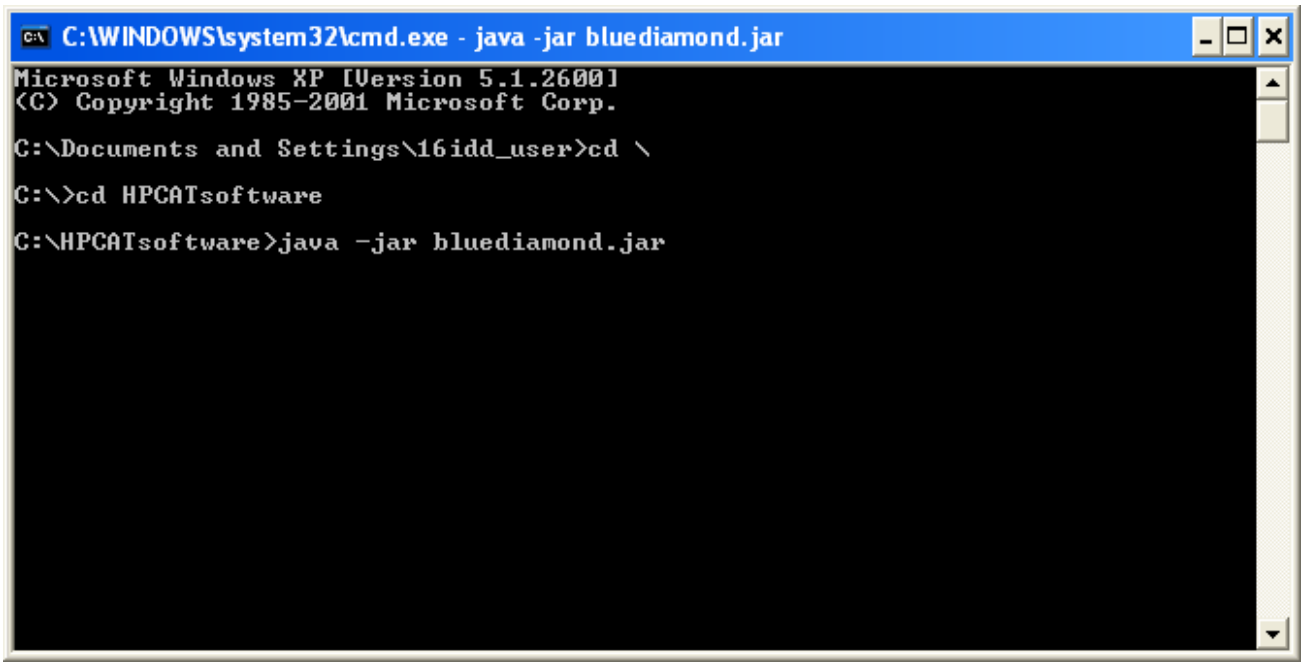
The Java-based **HPCAT Bluediamond** software has been updated recently, and used together with scanSee program, especially for DCM energy calibration and overlay several scans together.

Starting Blue Diamond from command line

1. Click Windows icon “start” at the left bottom corner, then click “run”



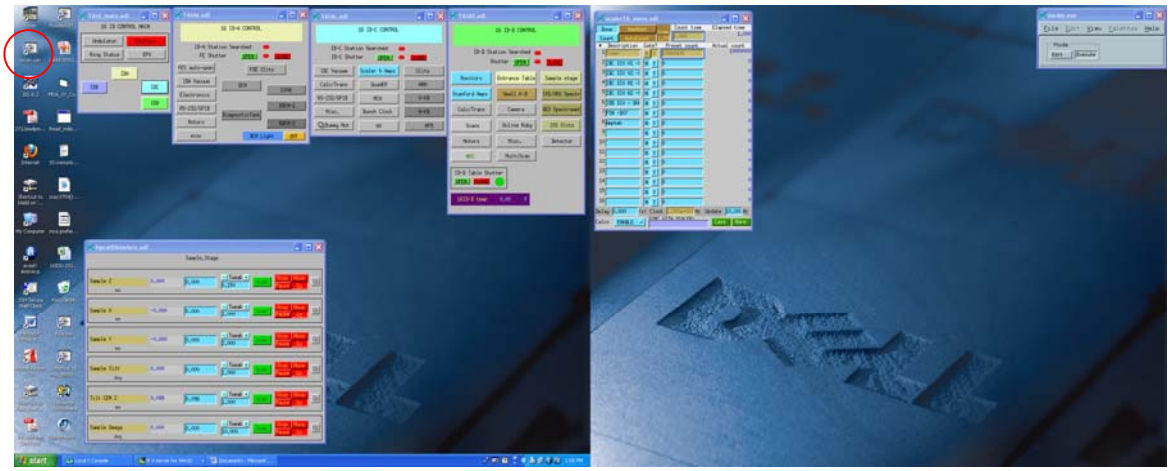

Run
Type the name of a program, folder, document, or Internet resource, and Windows will open it for you.
Open:
cmd
OK
Cancel
Browse...


C:\WINDOWS\system32\cmd.exe - java -jar bluediamond.jar
Microsoft Windows XP [Version 5.1.2600]
(C) Copyright 1985-2001 Microsoft Corp.
C:\Documents and Settings\16idd_user>cd \
C:\>cd HPCATsoftware
C:\HPCATsoftware>java -jar bluediamond.jar

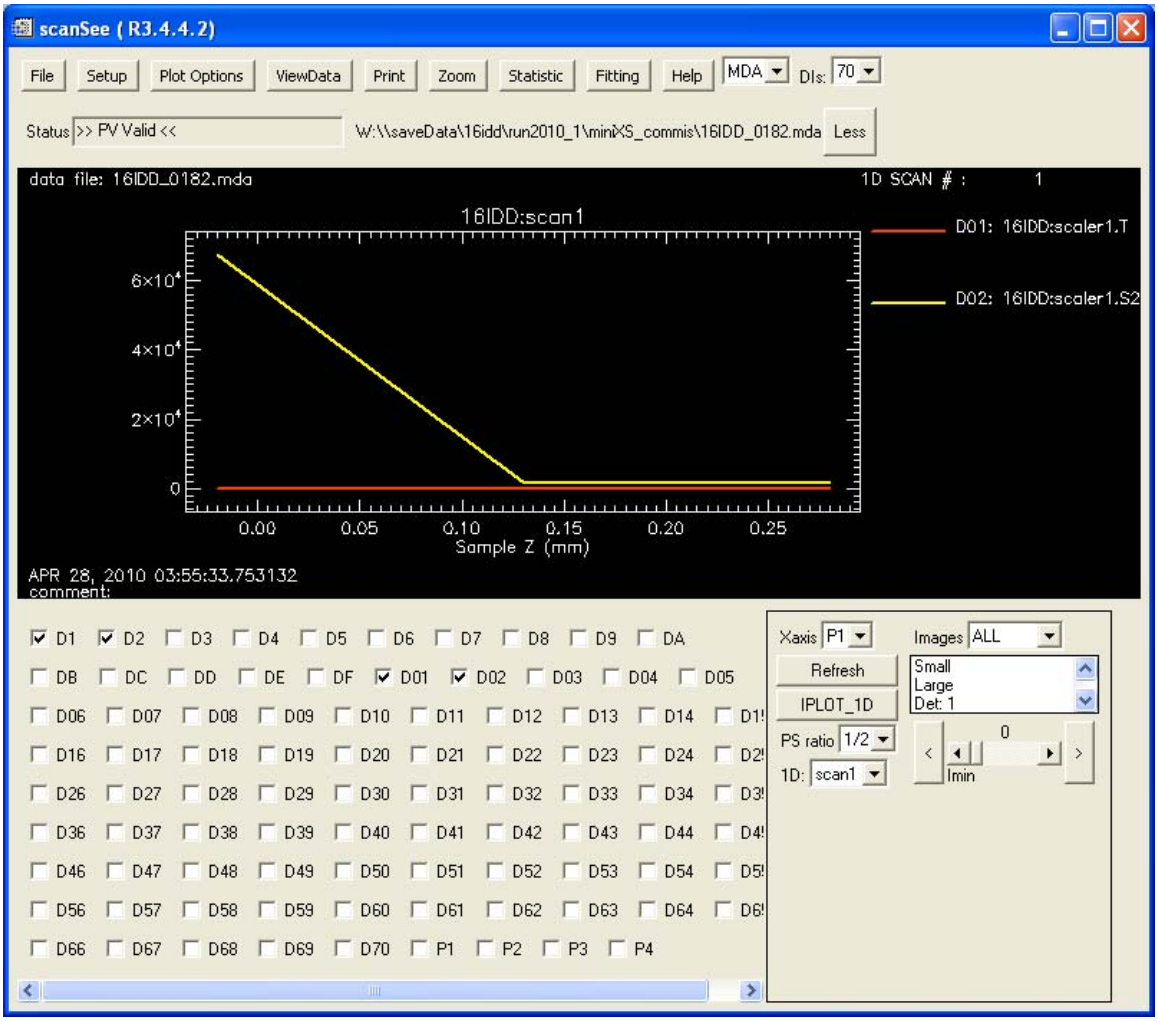
Every time when this software is started, user should specify the input configuration file “16IDD.txt” in the “C:\HPCATSoftware” directory. Note that this directory is local (not a network directory); however, any arbitrary configuration file in a network directory can be used if properly defined.
The software is straightforward to use and most of the menu items are self-instructing for real-time data display purposes.

IDL scanSee Software

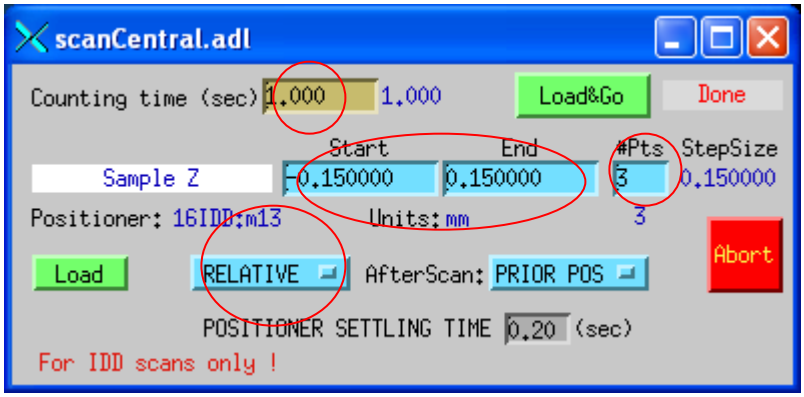
1. double click “sscan.sav”



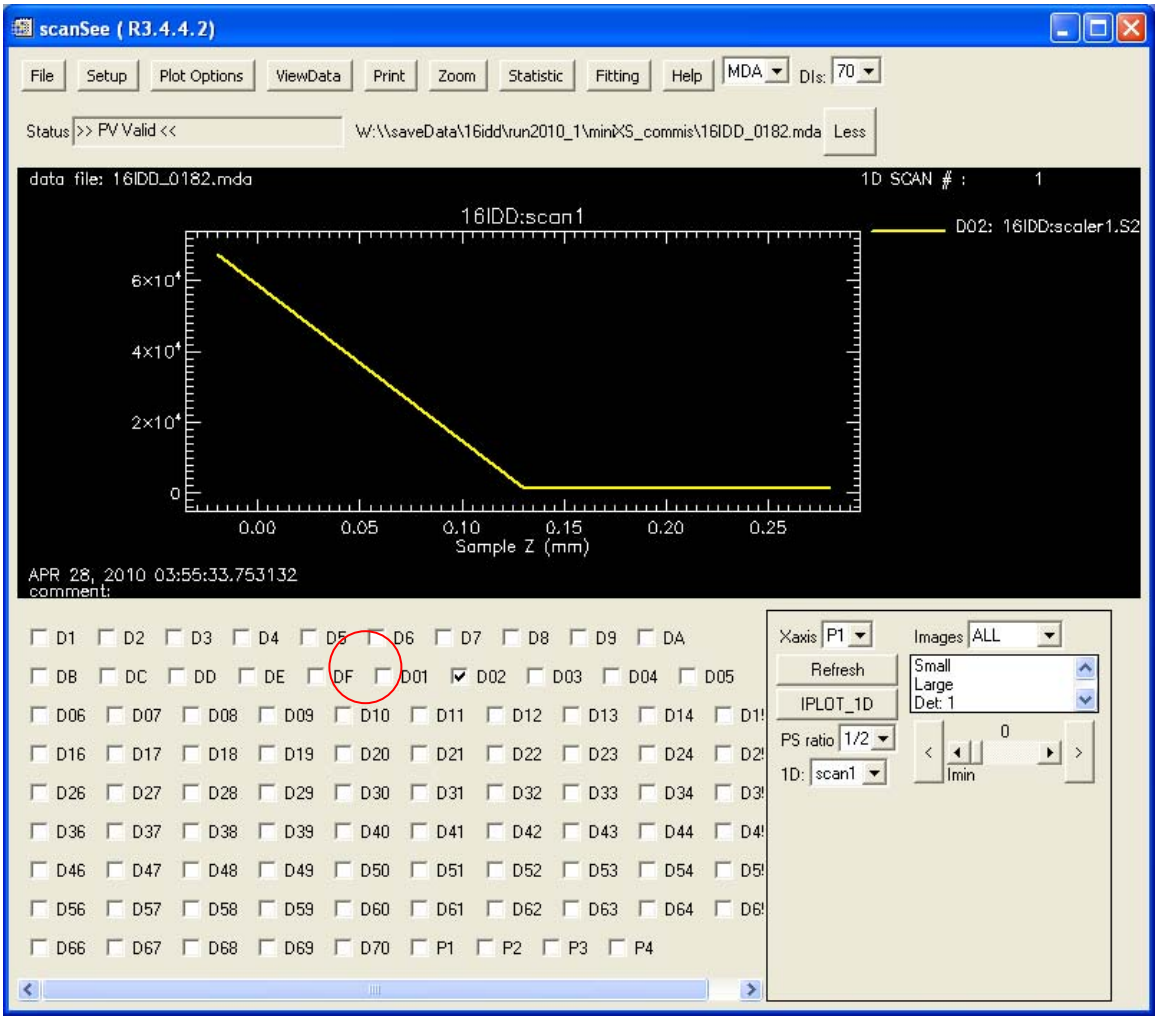
2. scanSee window will pop up



3. To start a scan, for example, Sample Z, setup scan range, counting time and number of points, then click “Load&Go”



4. To see the scan, click corresponding detector, for example, here D02 corresponds to IDC ion chamber V1

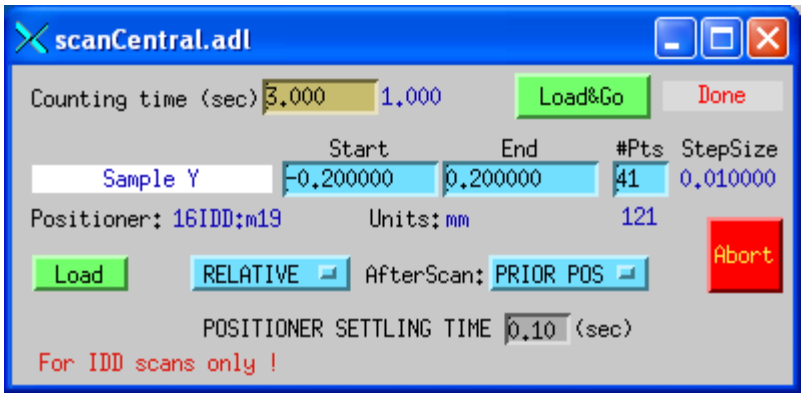


2D scans of Sample Absorption

We want to do a y- and z- scan against a PIN diode to align a sample.

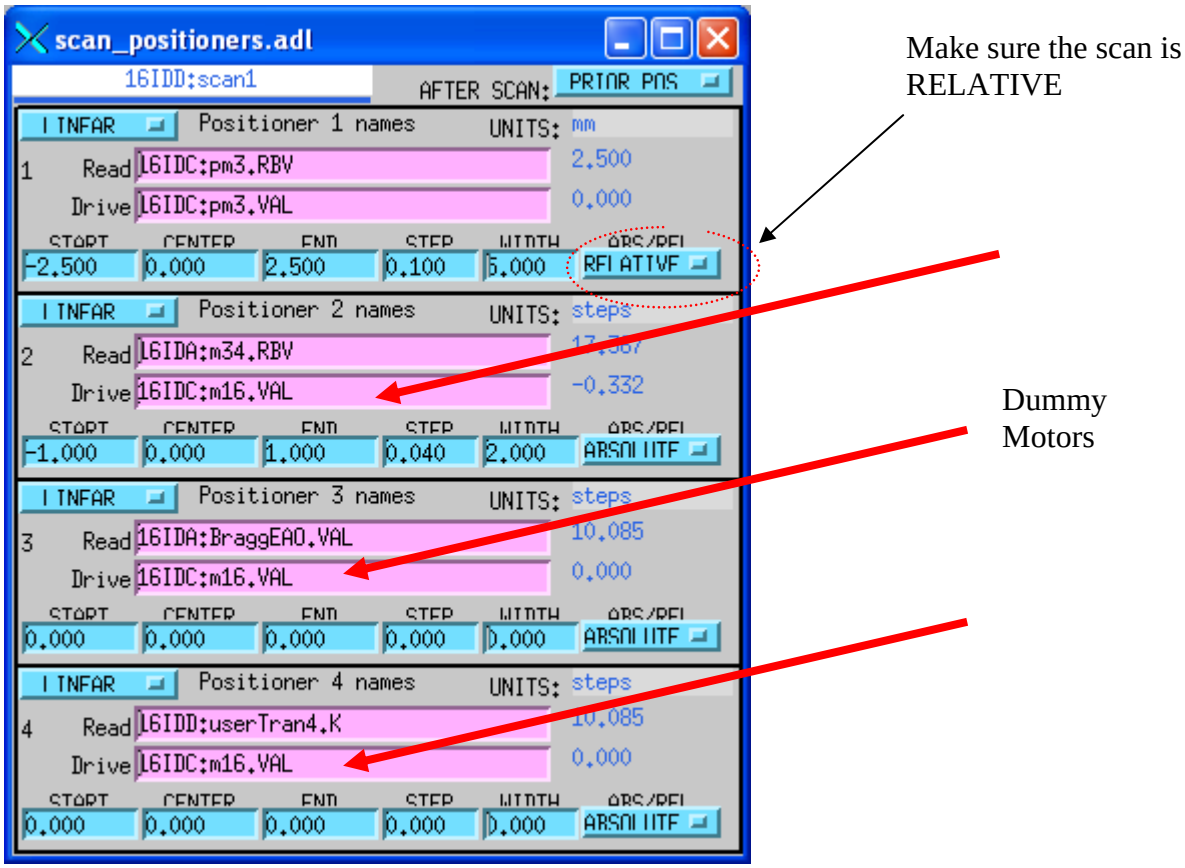
First set up the inner y scan by the scan module and only hit LOAD (NOT Load& Go)

SamY is the 'inside loop' 16IDD:m19.VAL



If you have dummy positioners which are written to the data file, but not scanned
Fill out the .VAL field with dummies

16IDC:m16.VAL so that the mda file has the correct format to be read by Arun's program



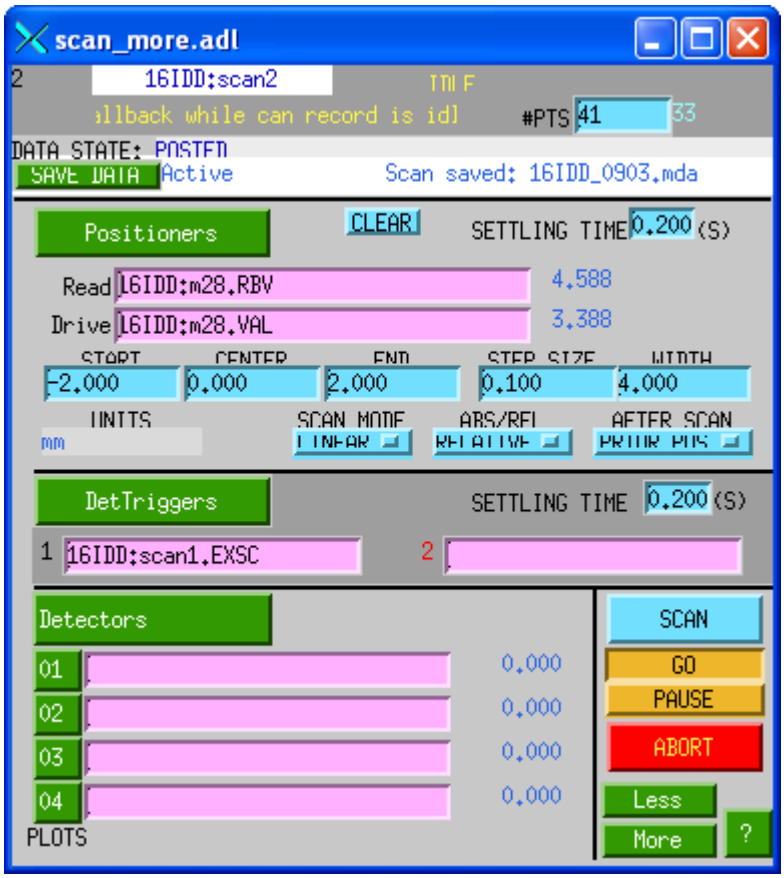
Make sure the scan is RELATIVE

Dummy Motors

Then go to the scan2 module

Typically, SamZ is the ‘outside loop’ 16IDD:m13.VAL

motor 28 is tilt center z for the z in this case
16IDD:m28.VAL



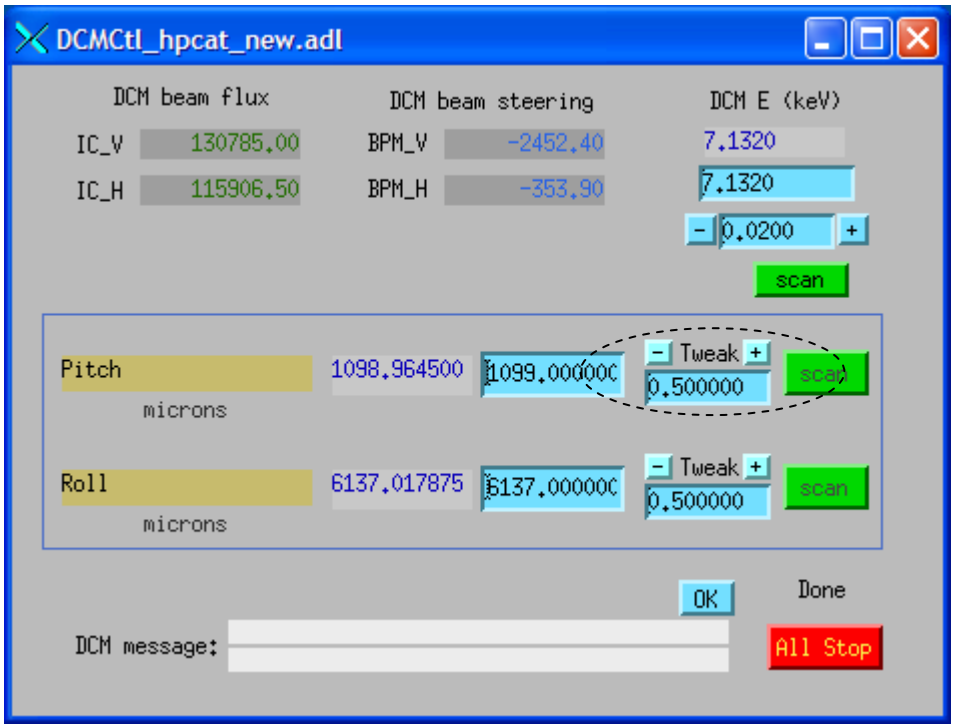
To execute the scan, hit the SCAN in the scan2 module.

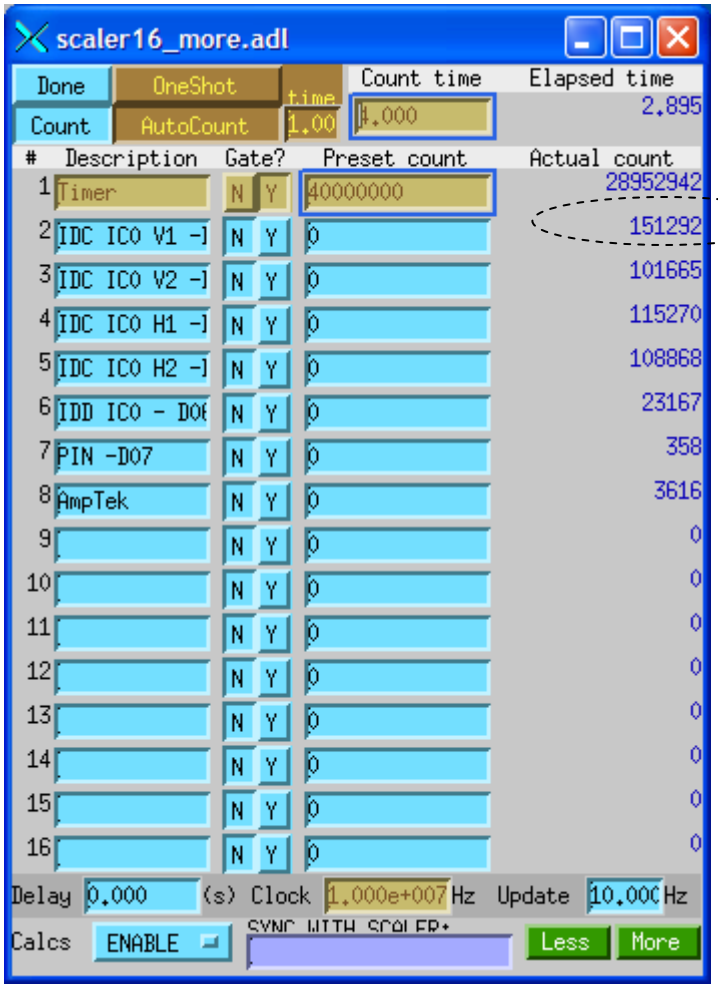
To graph, In scanSee, choose the ‘Det 7’ and click it, you should see the real time plot

The outside scan position value will show on the top of the plot

Steering beam procedure

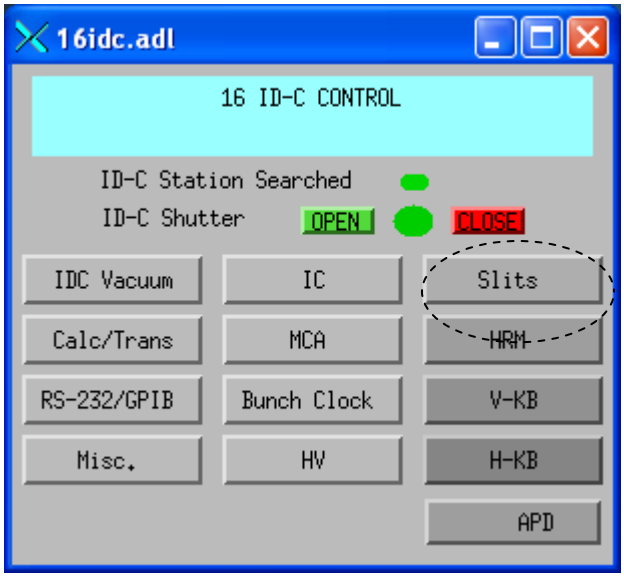
First tweak the pitch of the second crystal to optimize the countrate in the ion chamber





Find the present vertical and horizontal positions of the incident beam in IDC

Go to the IDC Slit window

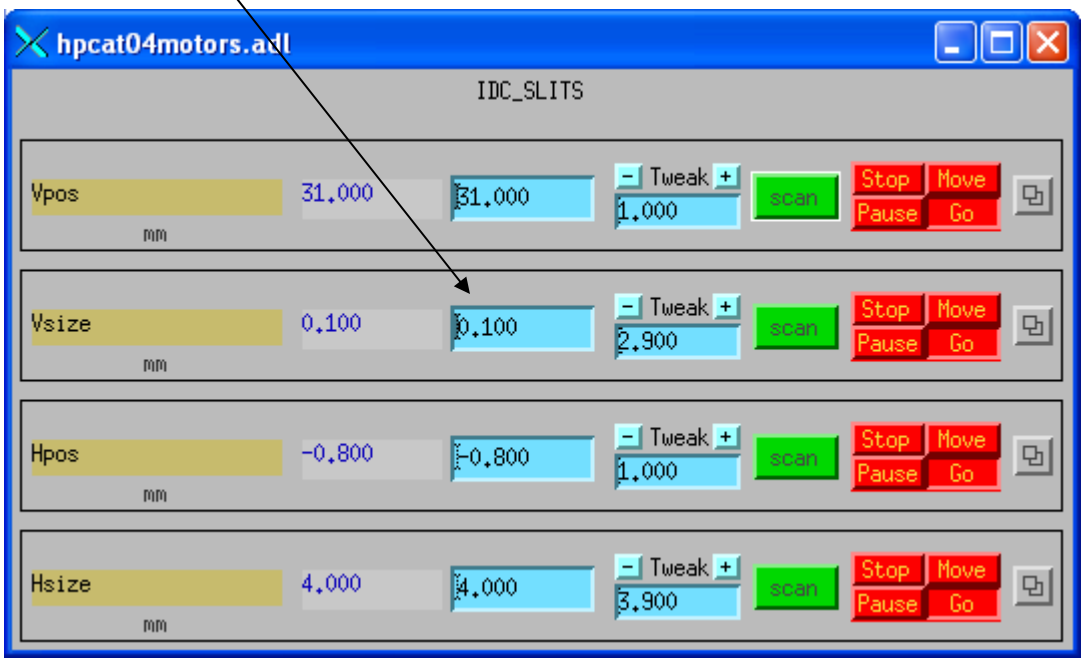


IDC vertical size = 2.5 when taking data

Close size to 0.1 mm

D03 plots the ion chamber counts after the vertical slit

Scan the IDC Vpos (Vertical position) to find the vertical position of the beam

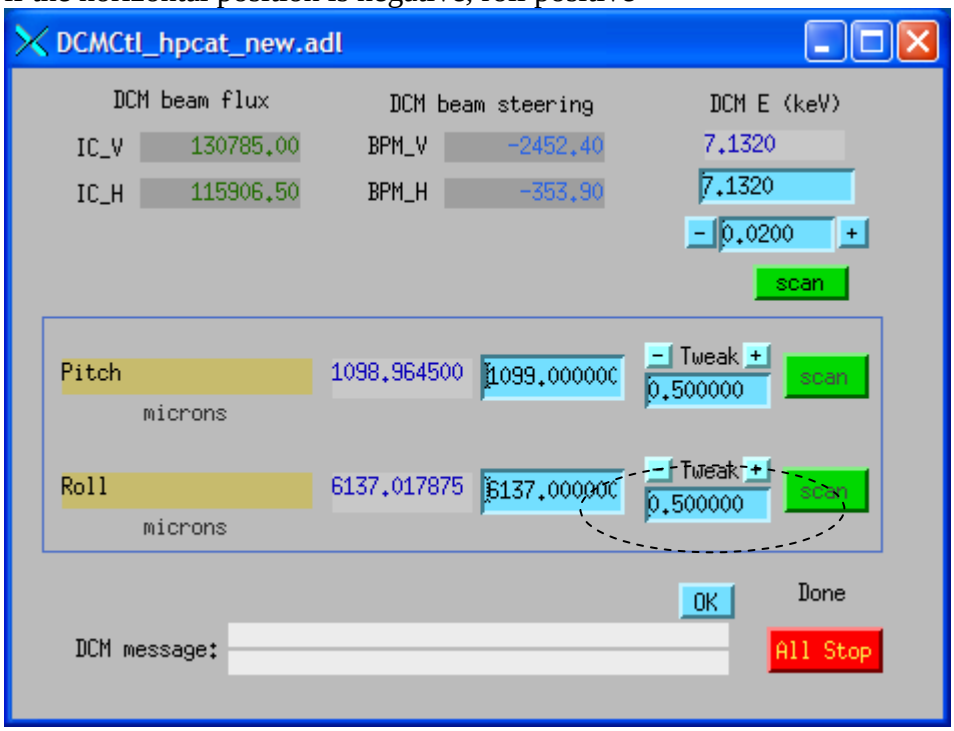


Note center of vertical position scan

then open IDC vertical slit to 2mm, close IDC horizontal to 0.1 (3mm when taking data)

scan horizontal slit position to find the center of horizontal position

if the horizontal position is negative, roll positive



scan horizontal slit position again, adjust roll until position within 50um

then open IDC horizontal slit to 3mm, then close vertical slit to 0.1, scan vertical slit position, if within 50um of position 35, it is ok, otherwise,

Now we will **move the vertical position of the beam** using an IDL program

Open IDL 6.3 icon
Go to ‘Files’
Go to ‘Recent Files’ and open

‘ DCM_Vertical_Vosition.pro’

Compile it (click the icon)
Run it (click the icon)
Input on the command line the vertical position you just found 31.46 return

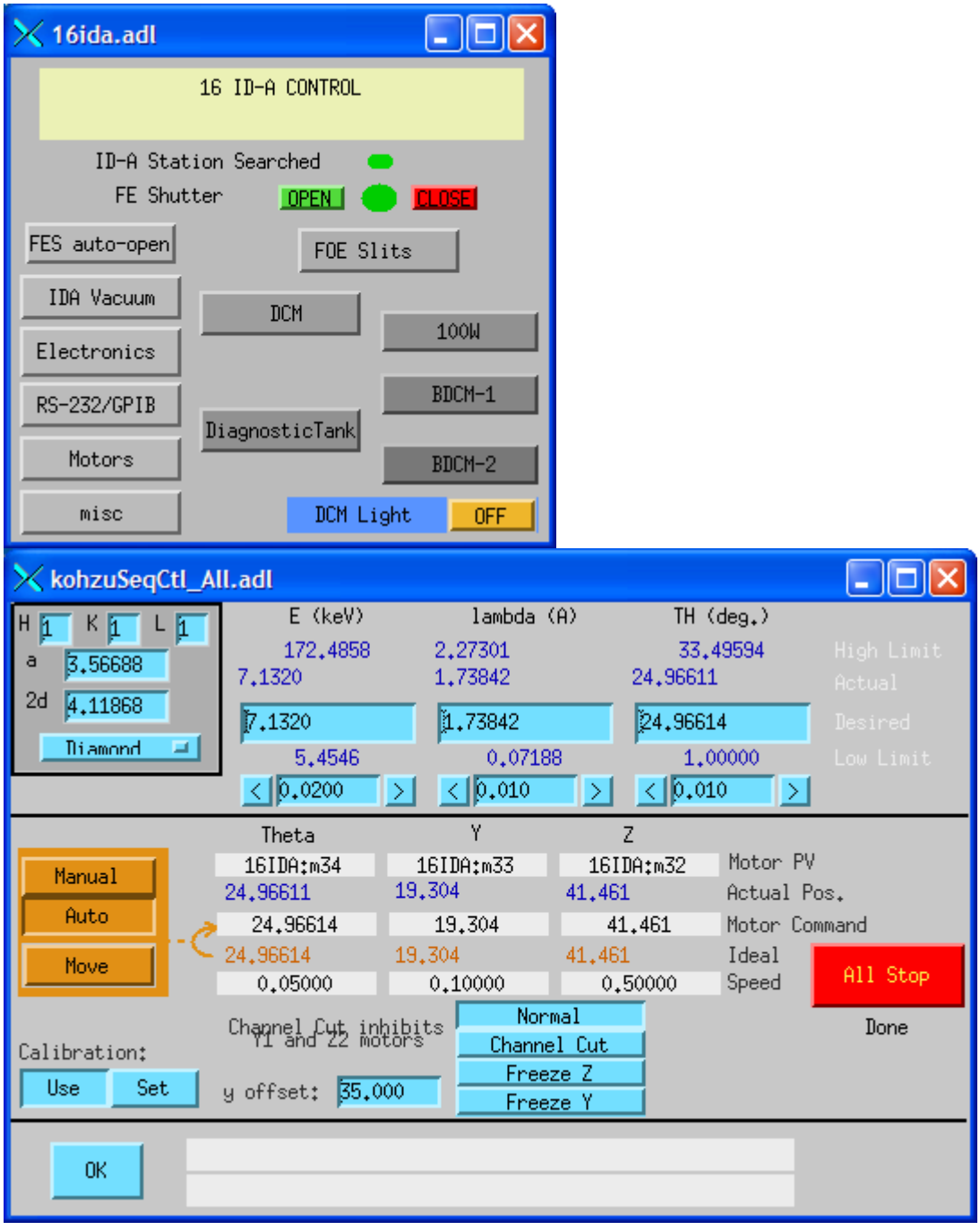
The macro will move the mono, and scan once again

The position of the beam should move to 35.00 mm (within 50 microns is fine)
If not then iterate by running the IDL program again

When the vertical position is within say 50 mircons of 35.000mm:

Make sure the Vsize opens back to 2.000 mm

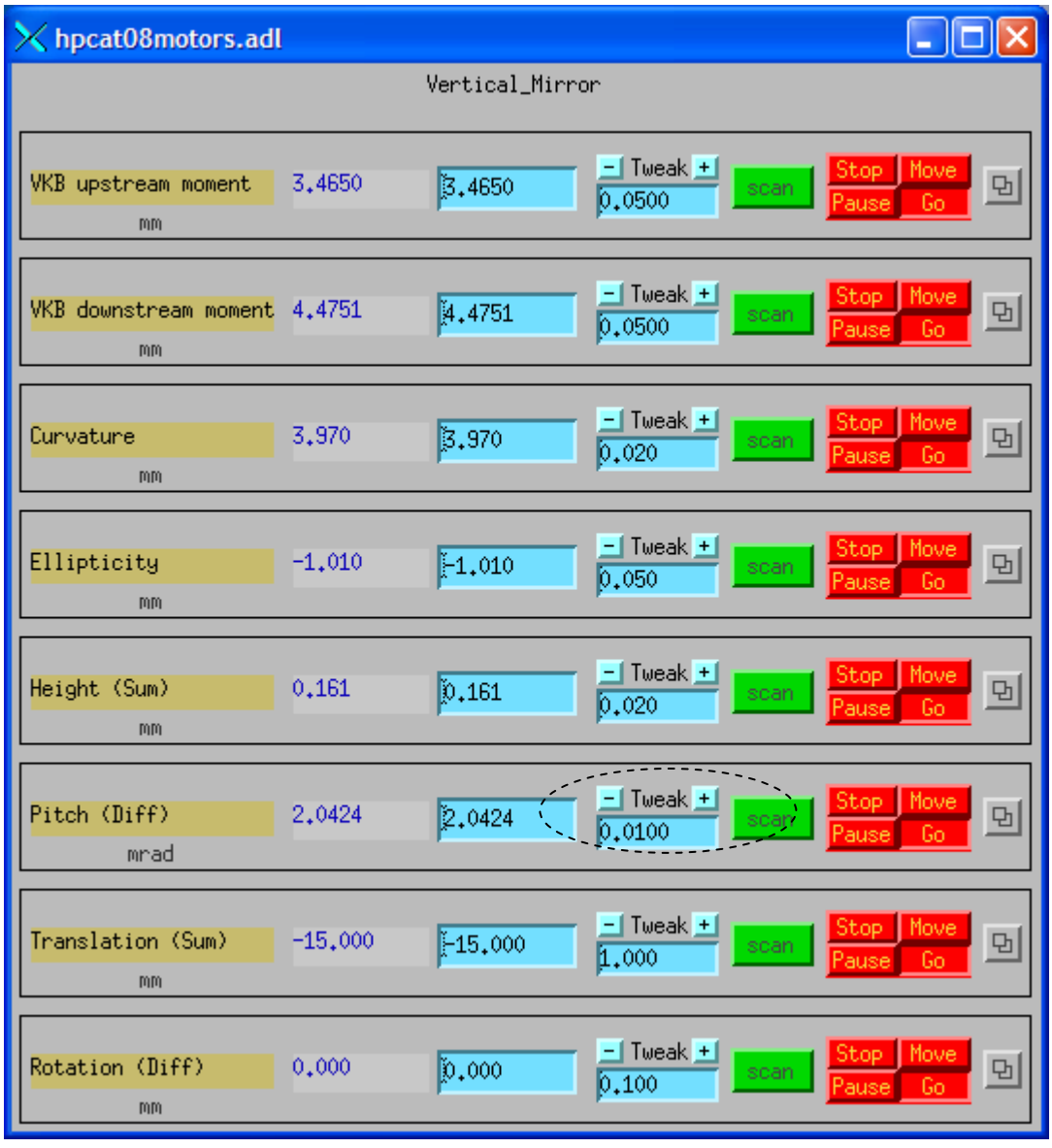
At this point we have finished moving the beam back to 35.000 at the IDC slits, then remember to reset the DCM



Click DCM, select "Full DCM Control", Click "Set", move mouse to energy window "7.112", press "enter", if it shows "done" then ok, otherwise, it shows "moving", then click "move", it will show "Done", then click "OK", then click "Use".

Steer beam through clean-up Pinhole

Even though the beam is in the correct place in IDC, the focused beam in IDD may not be going thru the cleanup pinhole, so need adjust VKB and HKB pitch by small step, for example, 0.001mrad to get maximum intensity in PID diode (had better remove sample from sample stage)

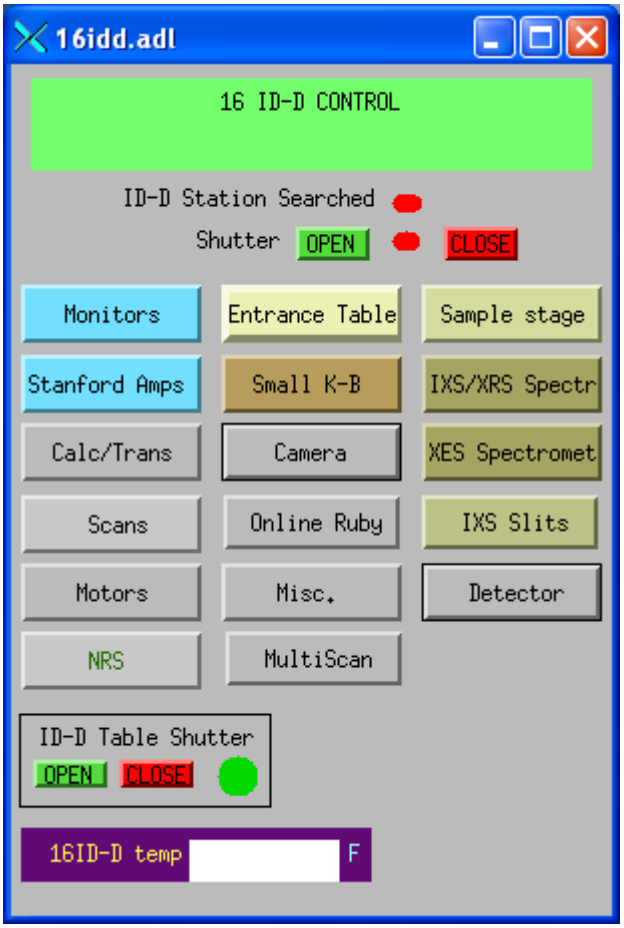


Realign the sample to make sure the beam hit the sample.

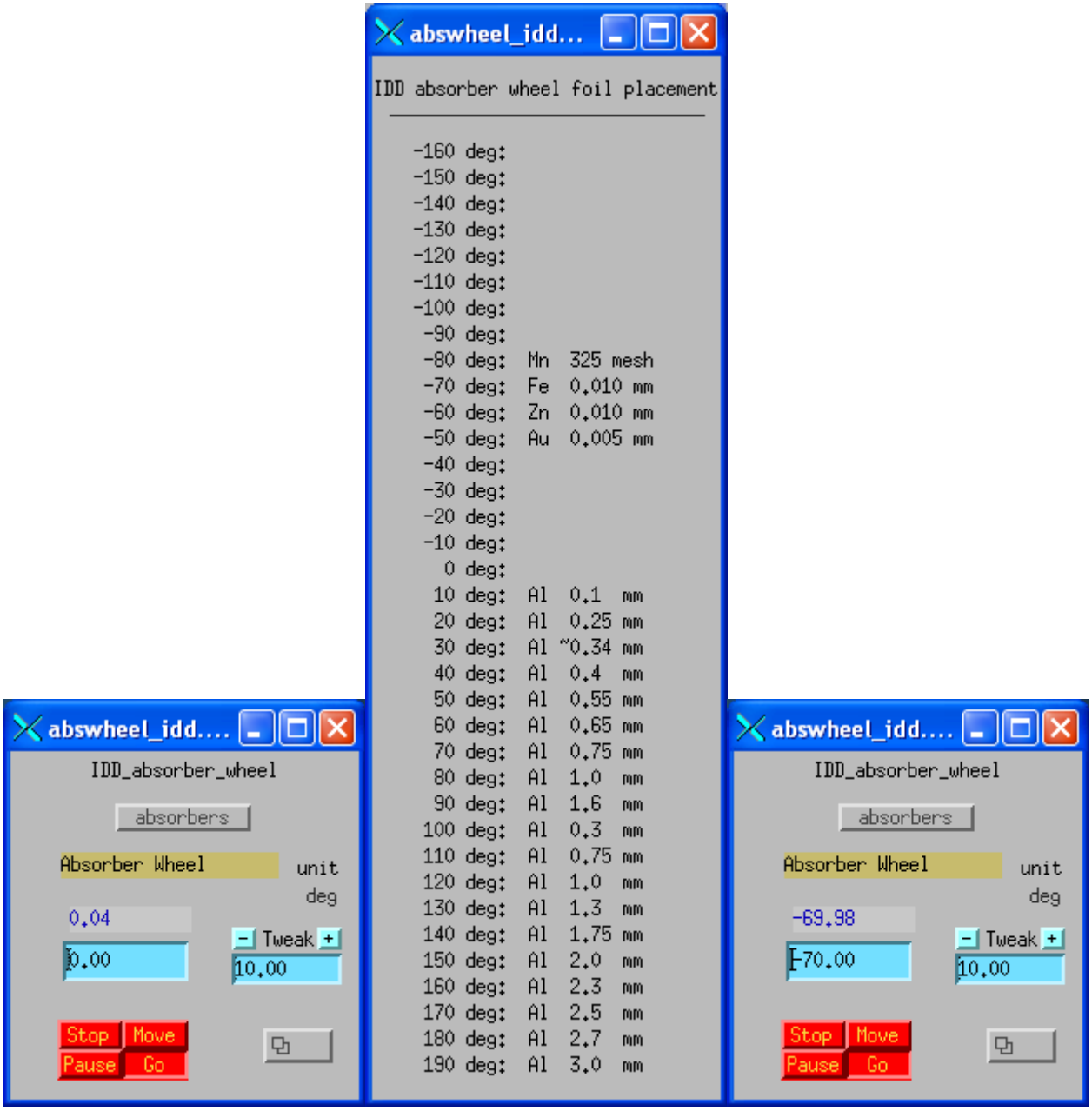
DCM Energy calibration using Foil

Using Fe foil energy calibration as an example

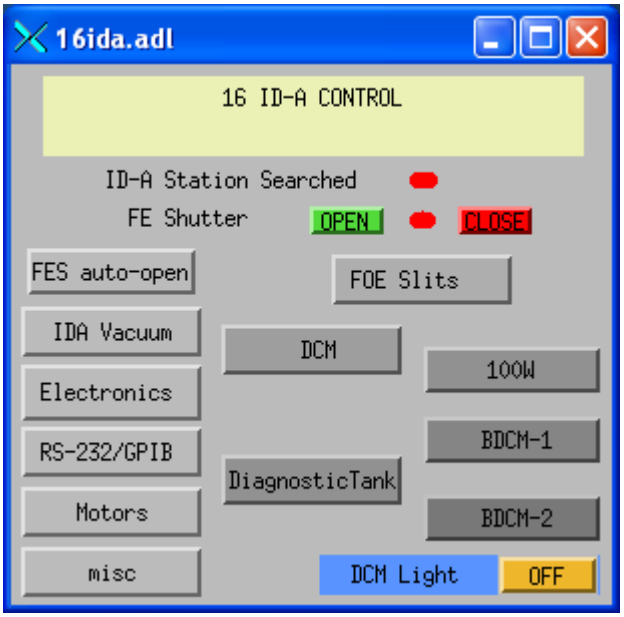
1. put IDD absorber wheel to -70 degree which is corresponding to Fe foil, if the foil you need is not in the wheel, you can put the wheel to 0 degree then attach your foil to the wheel using tape.



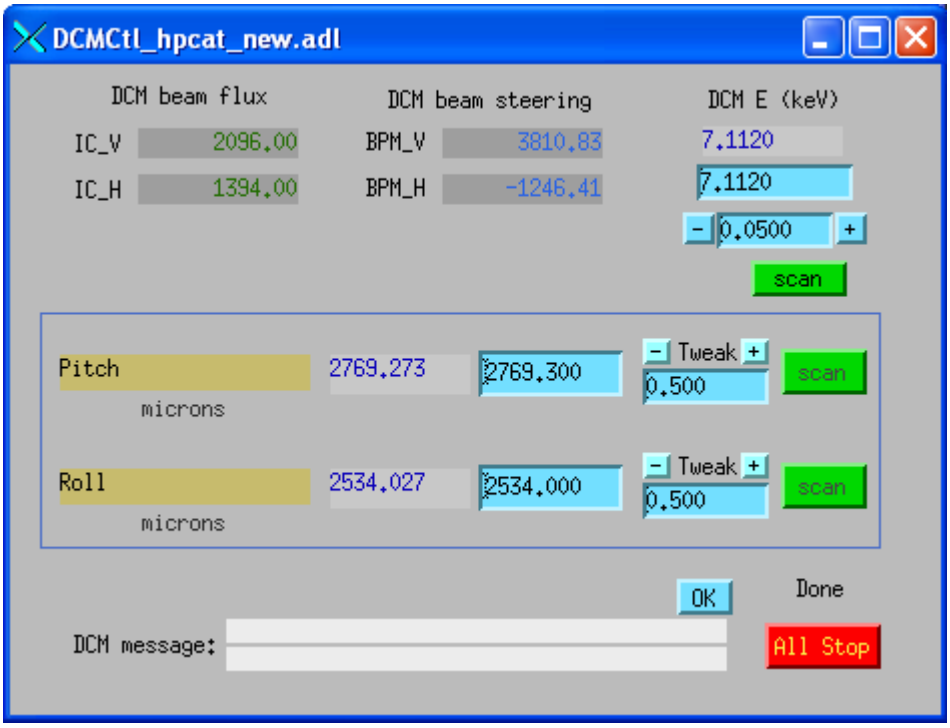
From “Entrance Table” to get Absorber wheel panel, put it at -70 degree for Fe foil, you can click “absorbers” to view correlation between angle and foil.



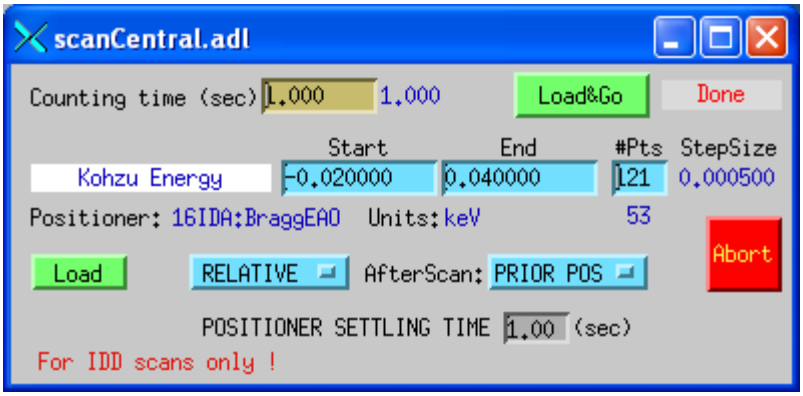
2. Scan DCM across 7.112keV (Fe k-edge)



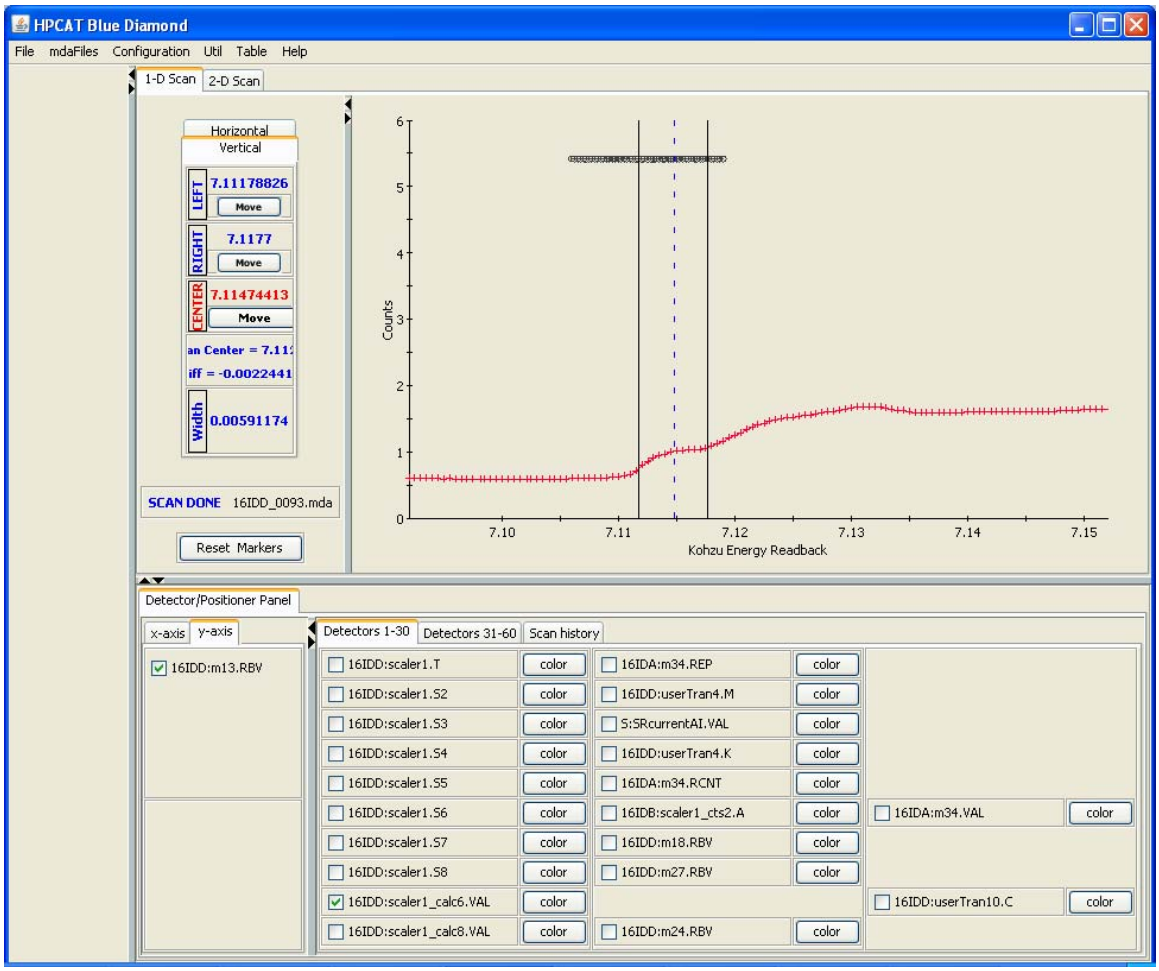
Click “DCM” and select “DCM Control New”



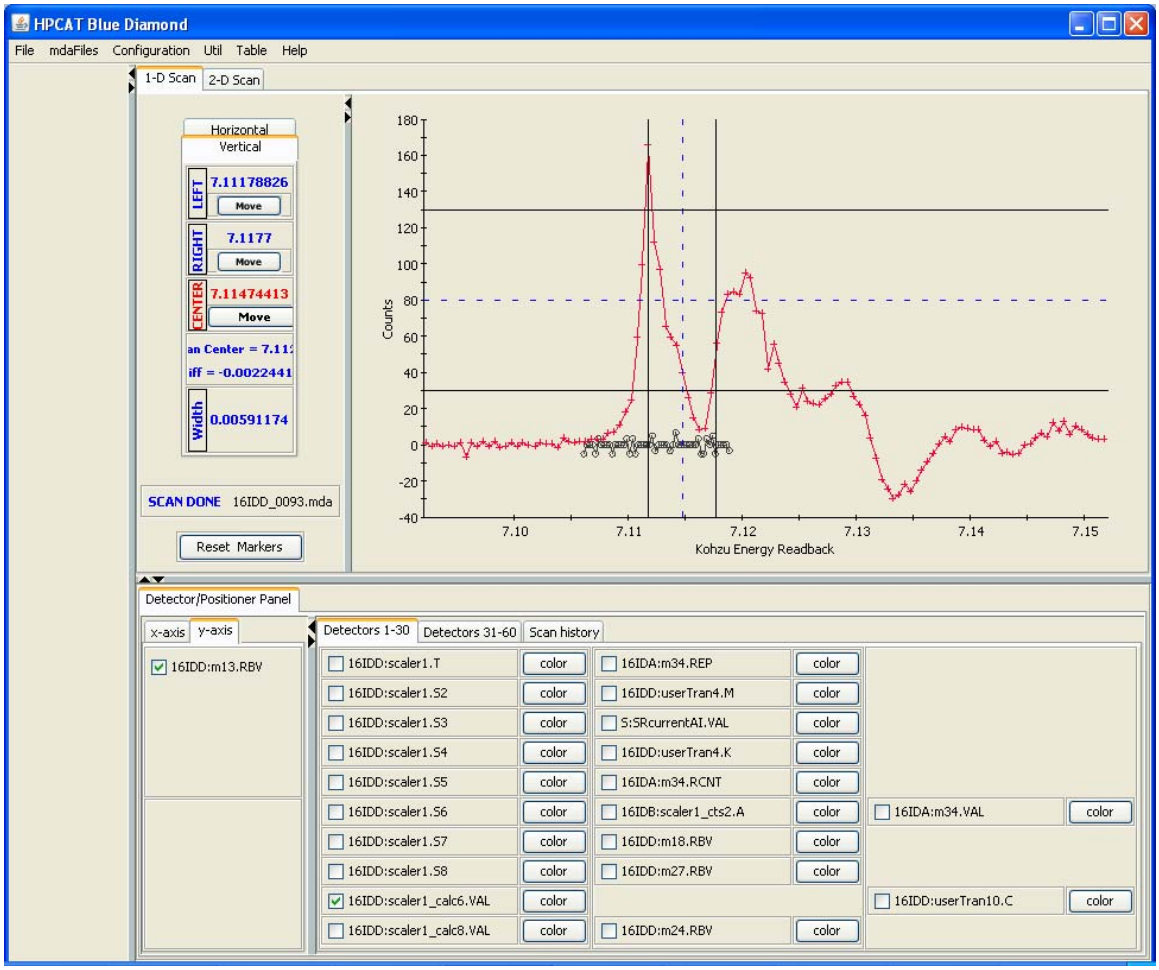
Click “scan”, then set up the scan range



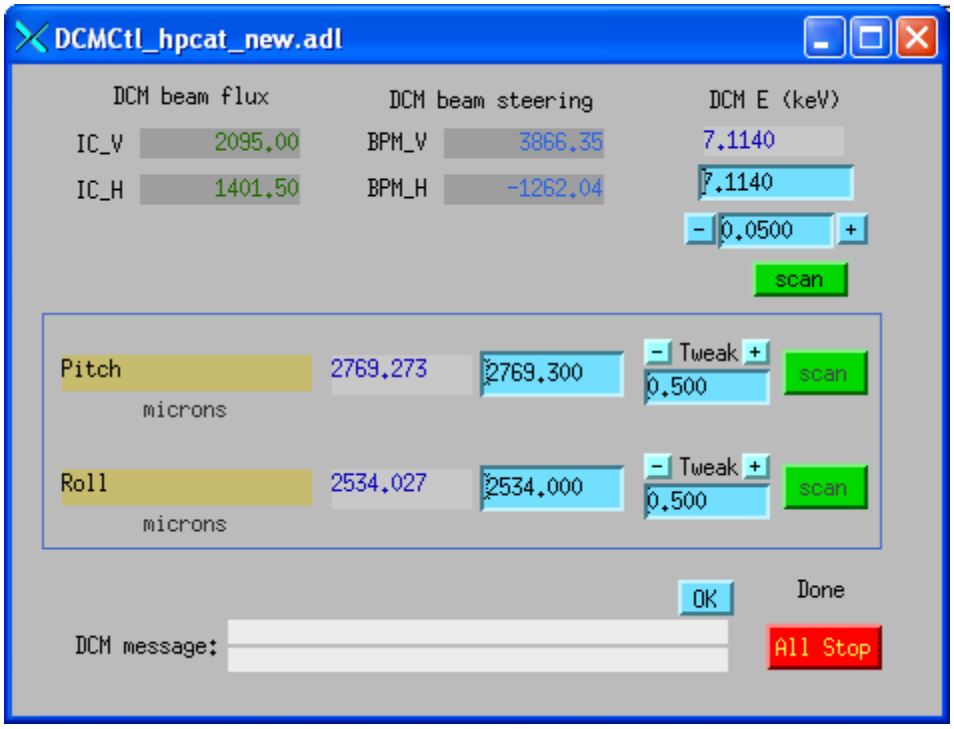
Click “Load&Go” to start the DCM energy scan



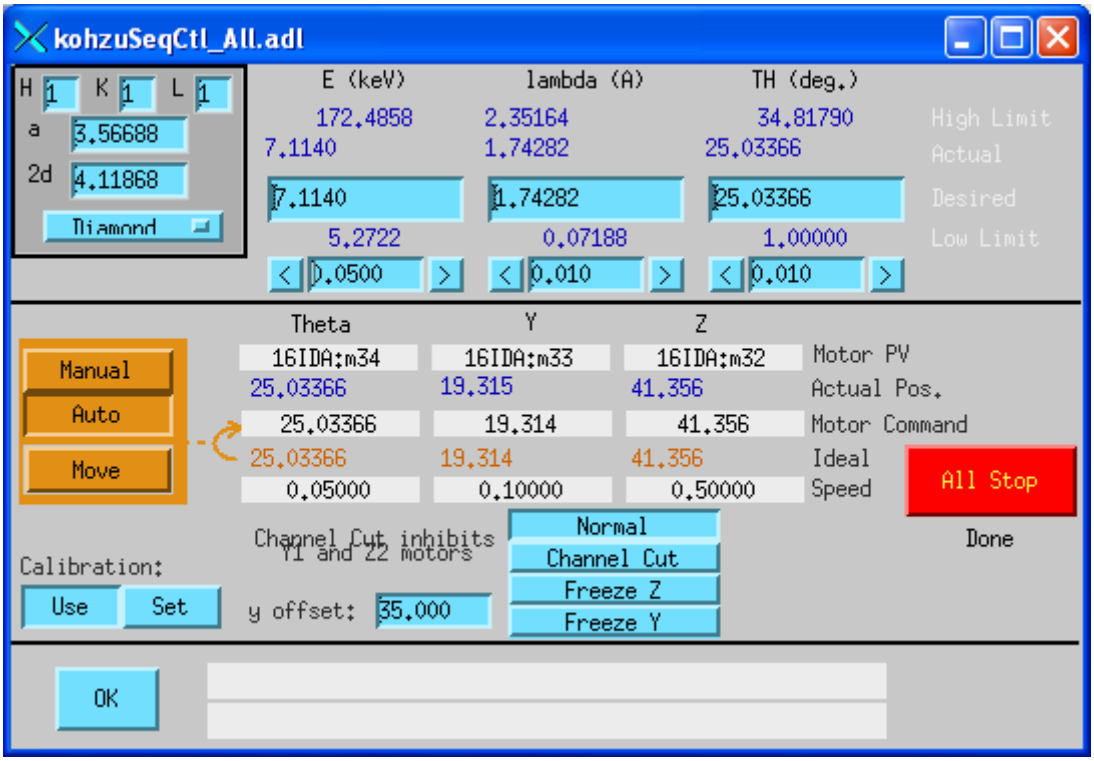
The red line here shows the DCM energy scan, click “Util” then select “Derivative”



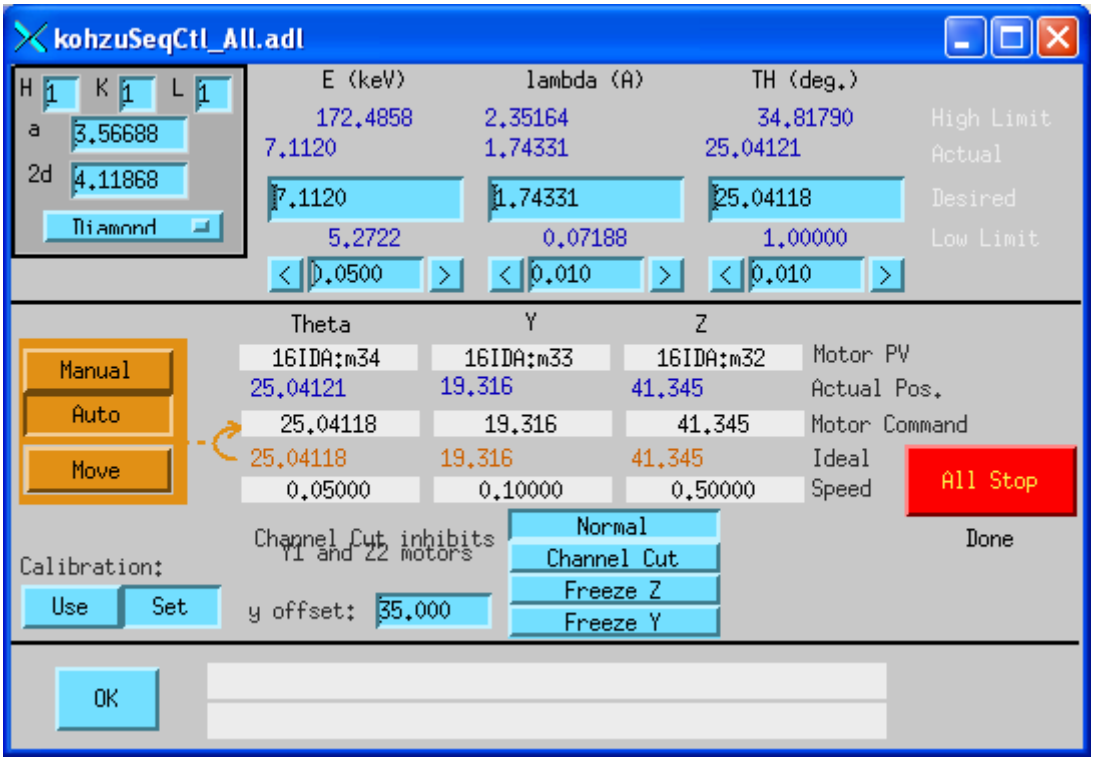
It shows the edge is at 7.1118keV which means the DCM energy is right. If the edge energy is different from tablet edge value, you need reset DCM energy. For example, if the scan shows the edge is at 7.114keV, then you first put DCM energy to 7.114keV



Then select “Full DCM Control” from “DCM” in 16 ID-A control



Click “set” and change 7.114 to 7.112keV

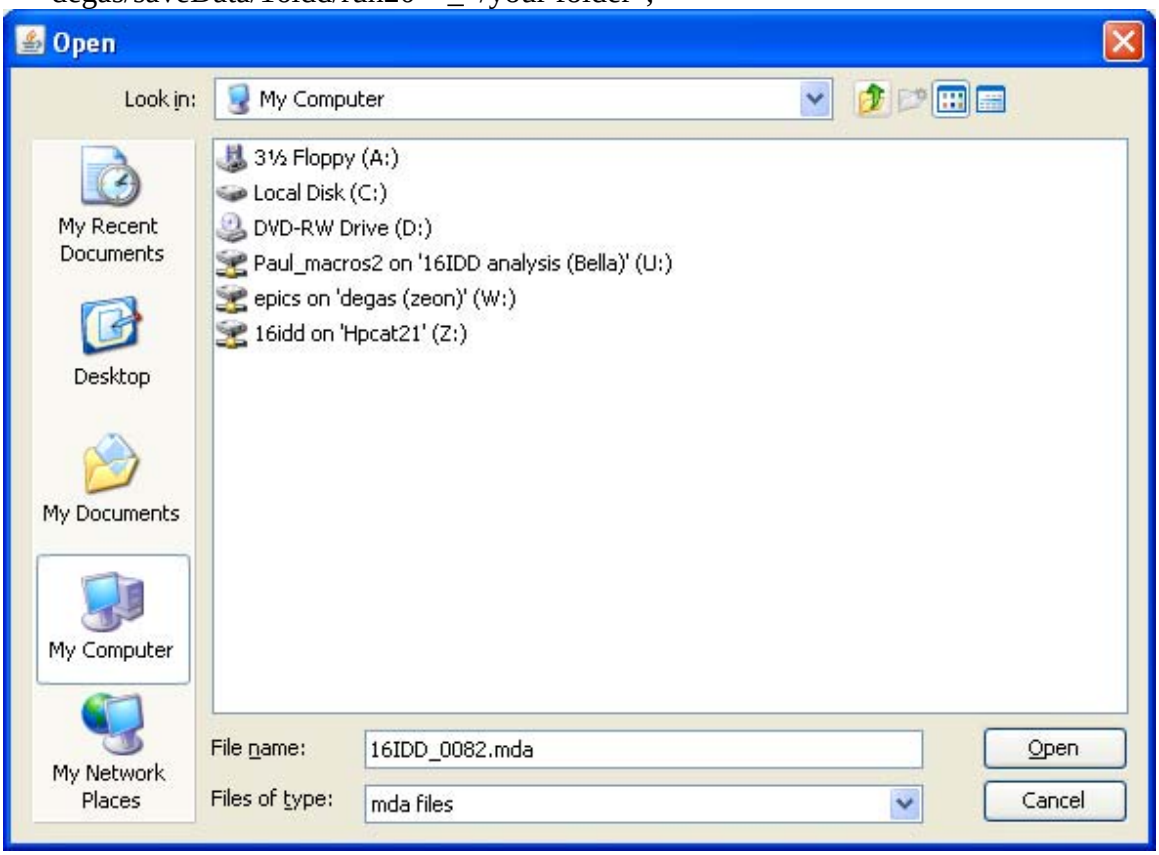


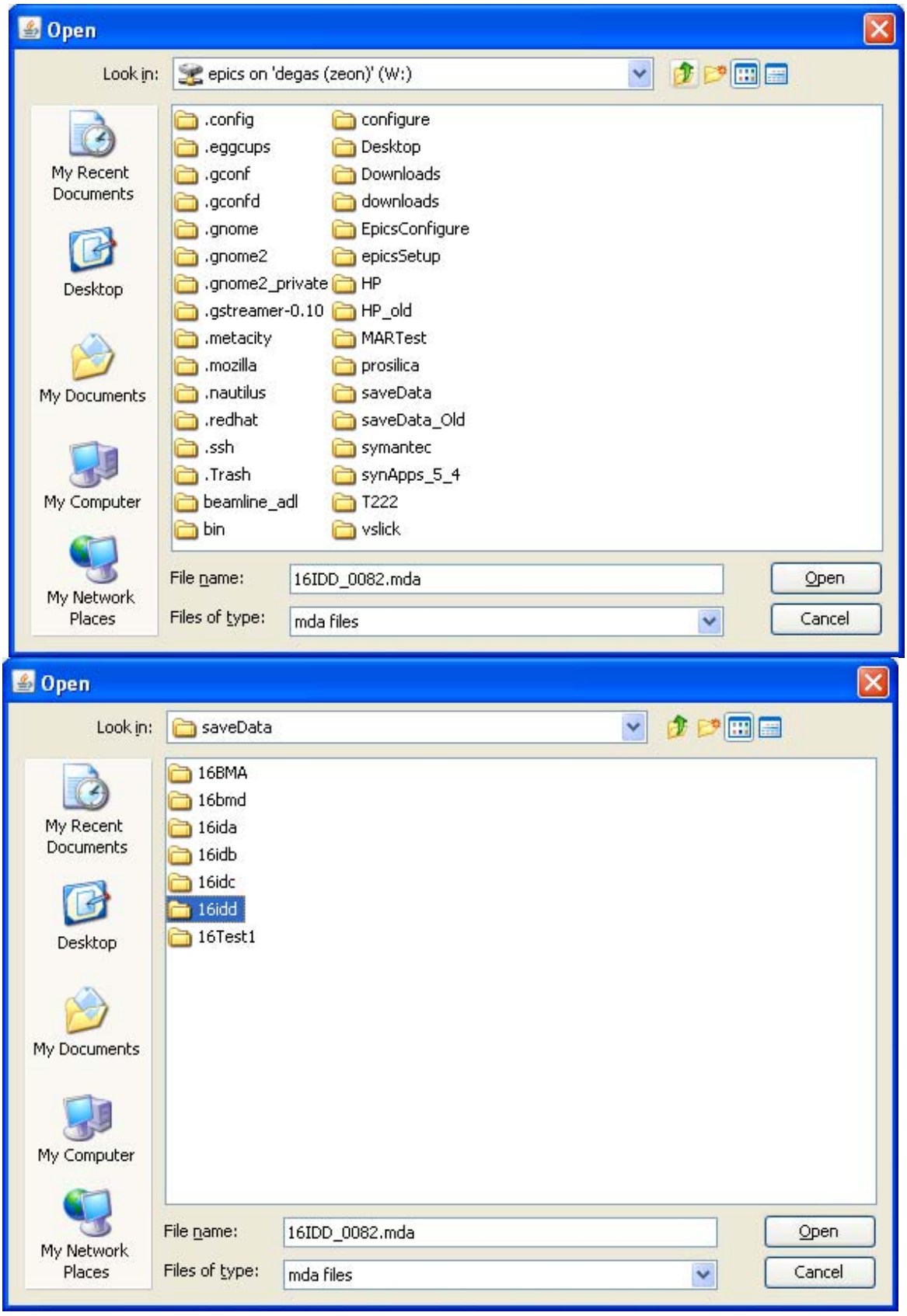
Remember to click “Use” to put DCM into function. You have reset DCM energy, it is better to re-do an edge scan to confirm the edge energy.

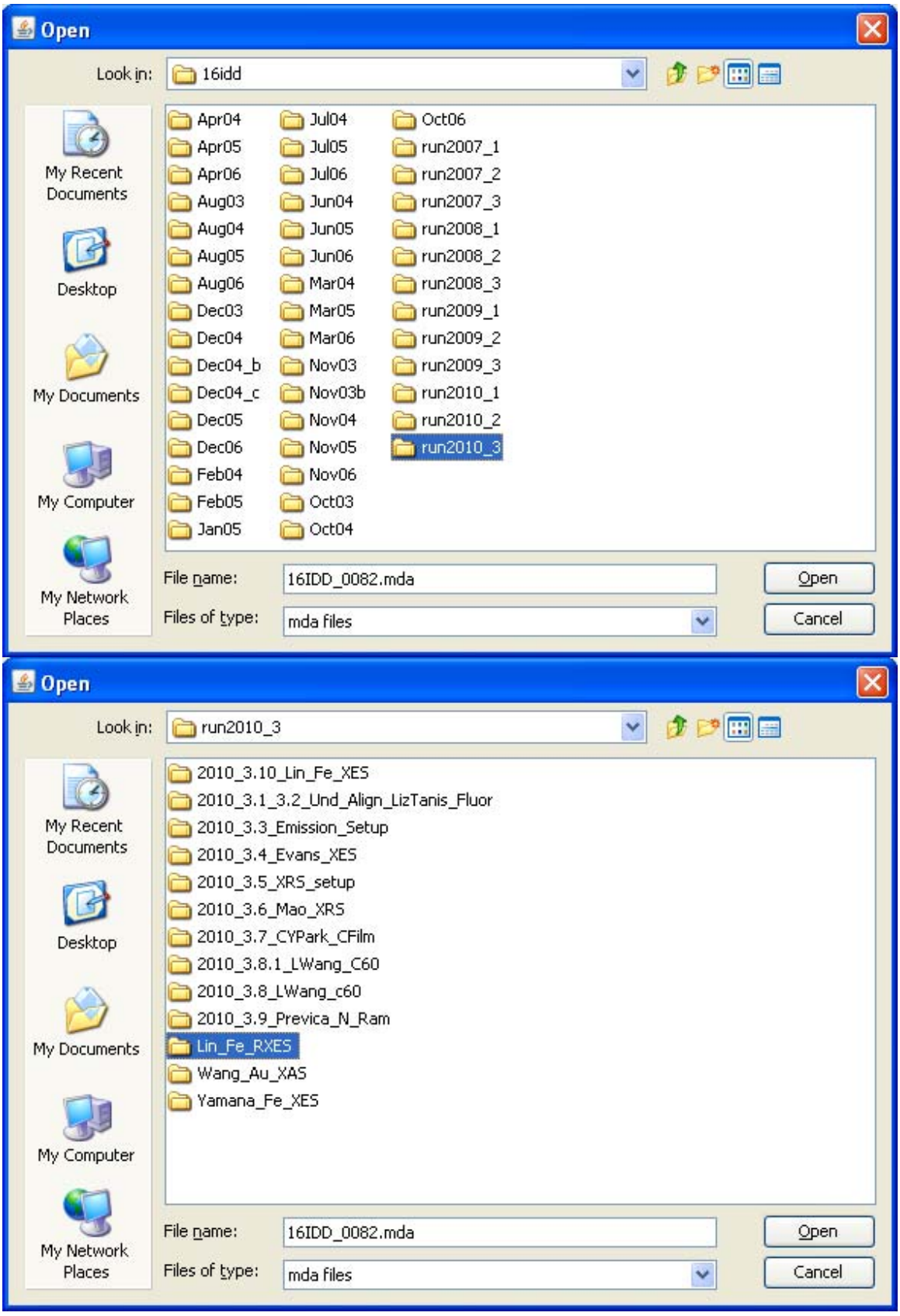
Overplot several scans in Bluediamond

You just finish a scan, for example, the following shows an energy calibration scan. You want to compare it to a similar scan you did before.

1. click “File”, then select “Open”, choose the right scan file to open. Normally the default folder is the folder where the mda file is saved. If not, please select the path “epics on degas/saveData/16idd/run20**_*/your folder”,




Open
Look in:
epics on 'degas (zeon)' (W:)
My Recent Documents
Desktop
My Documents
My Computer
My Network Places
.config
.eggcups
.gconf
.gconfd
.gnome
.gnome2
.gnome2_private
.gstreamer-0.10
.metacity
.mozilla
.nautilus
.redhat
.ssh
.Trash
beamline_adl
bin
configure
Desktop
Downloads
downloads
EpicsConfigure
epicsSetup
HP
HP_old
MARTest
prosilica
saveData
saveData_Old
symantec
synApps_5_4
T222
vslick
File name:
16IDD_0082.mda
Files of type:
mda files
Open
Cancel
Open
Look in:
saveData
My Recent Documents
Desktop
My Documents
My Computer
My Network Places
16BMA
16bmd
16ida
16idb
16idc
16idd
16Test1
File name:
16IDD_0082.mda
Files of type:
mda files
Open
Cancel


Open
Look in:
16idd
Apr04
Apr05
Apr06
Aug03
Aug04
Aug05
Aug06
Dec03
Dec04
Dec04_b
Dec04_c
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run2007_1
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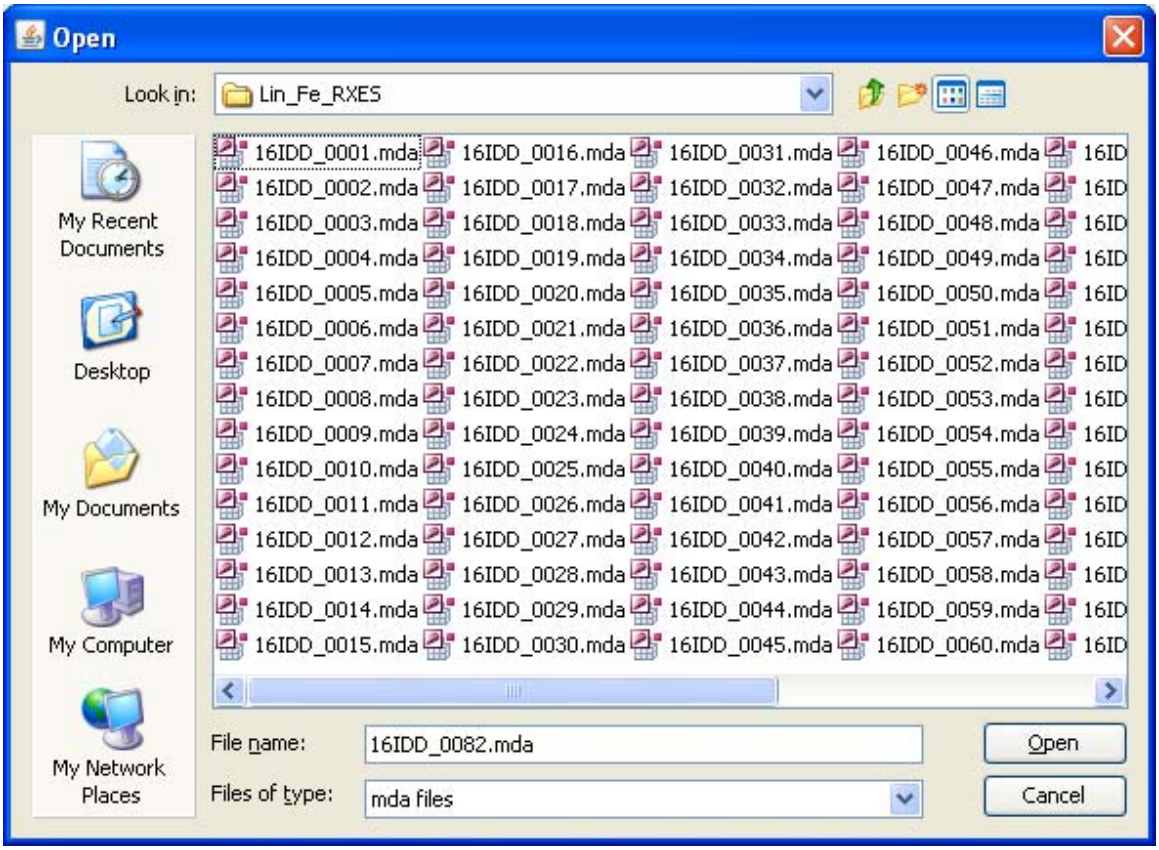
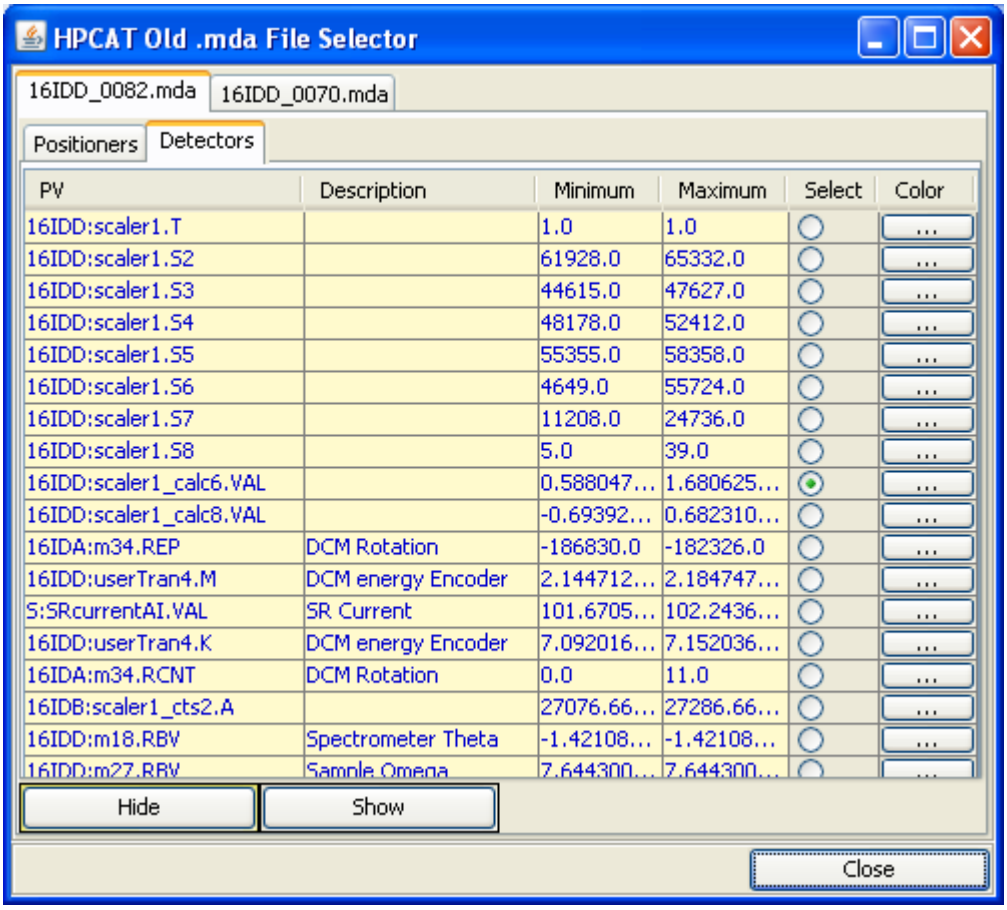
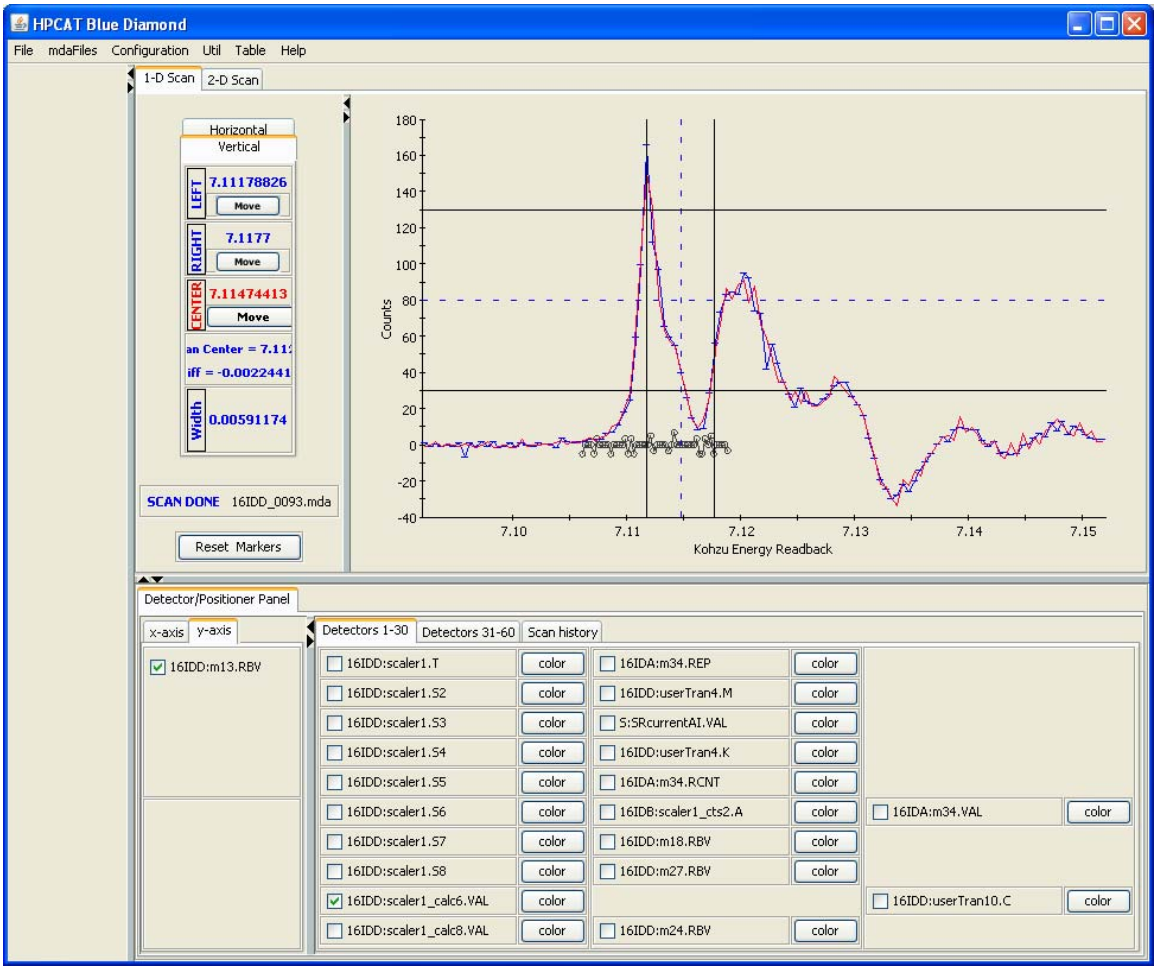
run2008_3
run2009_1
run2009_2
run2009_3
run2010_1
run2010_2
run2010_3
My Recent Documents
Desktop
My Documents
My Computer
My Network Places
File name:
16IDD_0082.mda
Files of type:
mda files
Open
Cancel
Open
Look in:
run2010_3
2010_3.10_Lin_Fe_XES
2010_3.1_3.2_Und_Align_LizTanis_Fluor
2010_3.3_Emission_Setup
2010_3.4_Evans_XES
2010_3.5_XRS_setup
2010_3.6_Mao_XRS
2010_3.7_CYPark_CFilm
2010_3.8.1_LWang_C60
2010_3.8_LWang_c60
2010_3.9_Previca_N_Ram
Lin_Fe_RXES
Wang_Au_XAS
Yamana_Fe_XES
My Recent Documents
Desktop
My Documents
My Computer
My Network Places
File name:
16IDD_0082.mda
Files of type:
mda files
Open
Cancel



2. select the file you want to open, for example here, 16IDD_0070.mda


HPCAT Old .mda File Selector
16IDD_0082.mda
16IDD_0070.mda
Positioners
Detectors
PV
Description
Minimum
Maximum
Select
Color
16IDD:scaler1.T
1.0
1.0
16IDD:scaler1.S2
61928.0
65332.0
16IDD:scaler1.S3
44615.0
47627.0
16IDD:scaler1.S4
48178.0
52412.0
16IDD:scaler1.S5
55355.0
58358.0
16IDD:scaler1.S6
4649.0
55724.0
16IDD:scaler1.S7
11208.0
24736.0
16IDD:scaler1.S8
5.0
39.0
16IDD:scaler1_calc6.VAL
0.588047...
1.680625...
16IDD:scaler1_calc8.VAL
-0.69392...
0.682310...
16IDA:m34.REP
DCM Rotation
-186830.0
-182326.0
16IDD:userTran4.M
DCM energy Encoder
2.144712...
2.184747...
S:SRcurrentAI.VAL
SR Current
101.6705...
102.2436...
16IDD:userTran4.K
DCM energy Encoder
7.092016...
7.152036...
16IDA:m34.RCNT
DCM Rotation
0.0
11.0
16IDB:scaler1_cts2.A
27076.66...
27286.66...
16IDD:m18.RBV
Spectrometer Theta
-1.42108...
-1.42108...
16IDD:m27.RBV
Sample Omega
7.644300...
7.644300...
Hide
Show
Close



Here scan82 and scan70 are overplotting.

Chapter

4

Software

Introduction

Data collection and data analysis software are available to users at ID-D beamline. As a rule please do not install any other software on these computers. If you do need to use your own software for data analysis, please contact the beamline staff and they will work with you to find a solution. Two PCs are provided at each experimental station to assist users in data collection and data analysis. In the next sections, data collection, data processing and general software available on these PCs is listed.

Software at Control Computer (16idd):

1. EPICS WIN32 Extensions
2. Hummingbird Connectivity V8.0
3. IDL 6.3
4. Microsoft Office 2003
5. PowerDVD5.7
6. SSH Secure Shell 3.2.
7. Adobe Reader 7.0
8. Symantec pcAnywhere
9. avast! Antivirus
10. Blue Diamond Version Aug. 17, 2009
11. OriginPro 7.0
12. Roxio (burn CD and DVD)
13. PowderDiffraction (by Wenge Yang)
14. ScanSee
15. MCA

Software at Data Analysis Computer (Bella):

1. EPICS WIN32 Extensions
2. Hummingbird Connectivity V8.0
3. Microsoft Office 2003
4. Roxio
5. IDL 6.2

6. SSH Secure Shell 3.2.9
7. Adobe Reader 8.0
8. Internet Explorer 7.0.5730.11
9. ION 6.4 (unknown distributor)
10. ImageJ 1.42q (seems to be an image processing software)
11. Fit2D V12.077
12. GIMP
13. EditPro (evaluation version)
14. IFeffit (for EXAFS)
15. OriginPro 7.0
16. Acrobat standard 6.0
17. Acrobat distiller 6.0
18. OpenOffice
19. XOP2.3
20. Picasa 2

Software at Focus Checking (hpcat36):

1. Mathematica 4.1
2. Microsoft Office 2003
3. OriginPro 7.0
4. Roxio
5. Sigmaplot 8.0
6. SSH Secure Shell
7. Acrobat standard 6.0
8. Acrobat distiller 6.0
9. WinView32
10. Roper Scientific